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Validation-Study Document

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Quick Urban and Industrial Complex (QUIC) CBR Plume Modeling System: Validation-Study Document

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1. Overview

This document contains information on QUIC validation studies that have been performed to evaluate the wind, pressure, and concentration solutions produced by QUIC. Tests of QUIC's source term models and specialized transport mechanisms (e.g., buoyancy algorithms, particle settling and deposition, liquid pool growth, droplet and pool evaporation) are also provided. A brief description of the experiment, a few example validation results, and references to journal articles, reports, and/or presentations are given. Both LANL and non-LANL sources are provided.

2. QUIC Pressure Solver

The QUIC-computed pressure field has been evaluated against several wind-tunnel experiments in which pressure was measured on buildings of different shapes and arrangements. Since the pressure field on the building surfaces is dependent on the local wind field near the wall, evaluation of the pressure field is considered a surrogate test for obtaining the correct strength and direction of the near-building recirculation patterns. A description of the pressure solver equations and solution methods can be found in:

Gowardhan, A.A., Brown, M.J. and Pardyjak, E.R.: 2009: Evaluation of a Fast Response Pressure Solver for Flow around an Isolated Cube, Environ Fluid Mech, vol. 10, no. 3, 311-328.

2.1 Cubical Buildings

Gowardhan, A.A., Brown, M.J. and Pardyjak, E.R.: 2009: Evaluation of a Fast Response Pressure Solver for Flow around an Isolated Cube, Environ Fluid Mech, vol. 10, no. 3, 311-328.

Summary: qualitative and quantitative evaluation of pressure contours on front, back, top, and side walls was conducted. Overall agreement was fairly good, and fell within the range of results of more computationally-intensive CFD codes. The version of QUIC used in this study did not have a side-wall recirculation algorithm, hence the performance on the side wall was poor.

Example results:

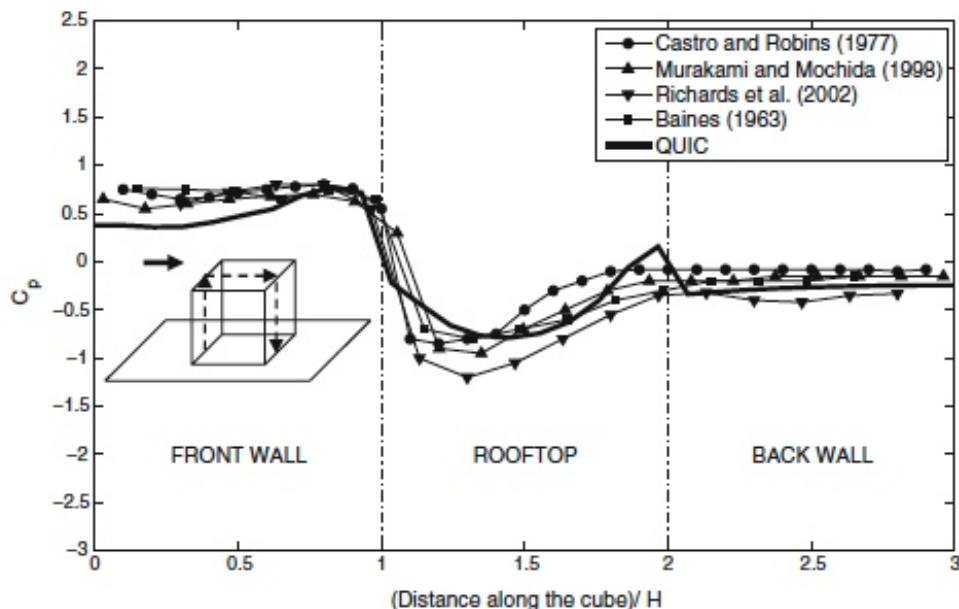


Fig. 8 Wind-tunnel measurements and QUIC Pressure Solver calculations of C_p for a cubical building with a power-law inflow perpendicular to the building face

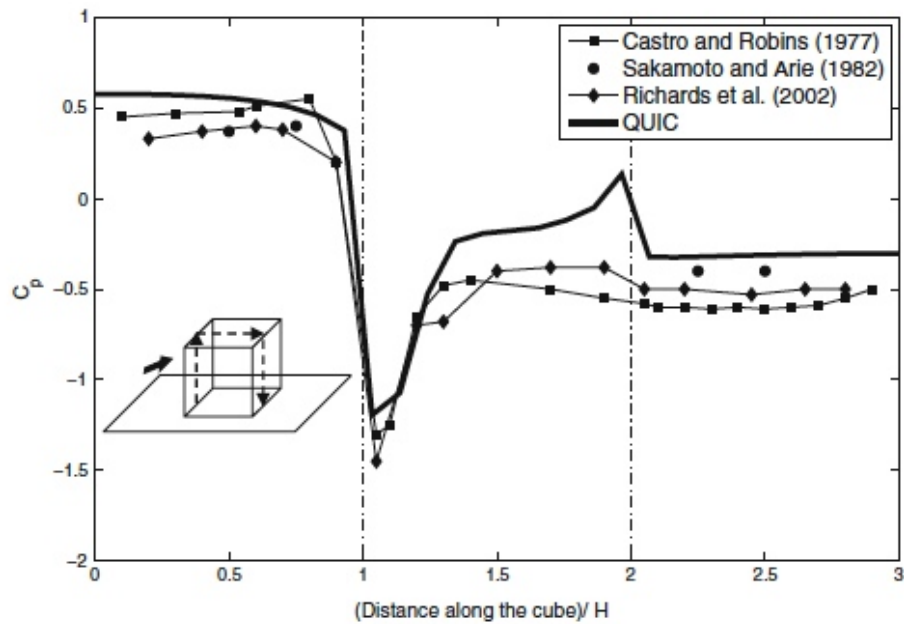


Fig. 11 Wind-tunnel measurements and QUIC Pressure Solver calculations of C_p for a cubical building with a power-law inflow winds at 45° to the cube

Other sources:

Gowardhan, A., 2008: *Towards understanding complex flow phenomenon in urban areas using numerical tools*, Ph.D. dissertation, University of Utah, UT.

Gowardhan, A., M. Brown, D. DeCroix, 2005: *Evaluation of the QUIC Pressure Solver: Comparison to wind-tunnel measurements on cubical buildings*, AMS ASAAQ San Francisco, LA-UR-05-2001, 13 pp.

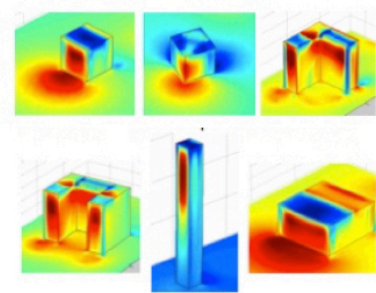
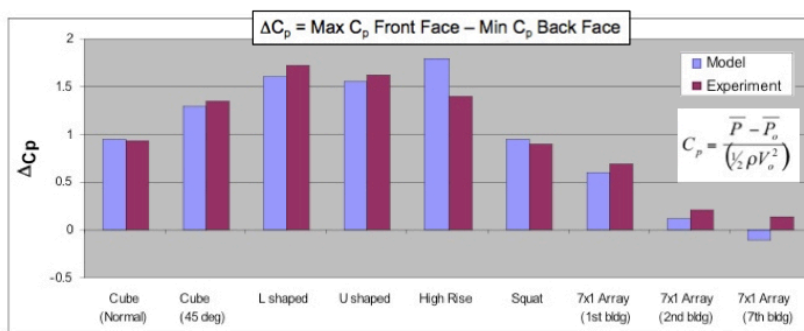
Gowardhan, A., 2005: *QUIC Pressure Solver – Description and comparison to experiments*, 31 pp.

2.2 Different-shaped Buildings

Brown, M., A. Gowardhan, E.R. Pardyjak, 2007: *Evaluation of a fast-response pressure solver for a variety of building shapes and layouts*, AMS 7th Symp. Urban Environment., San Diego, CA, paper 12.6, 4 pp.

Summary: qualitative and quantitative evaluation of pressure contours on high-rises, L- and U-shaped buildings, and idealized arrangements of grouped buildings was undertaken. Overall agreement was fairly good.

Example results:



Comparison of the pressure coefficient difference computed by QUIC-Pressure and measured in different wind-tunnel experiments for a variety of building shapes.

Other sources:

Gowardhan, A., M. Brown, M. Nelson, E. Pardyjak, D. DeCroix, D., 2006. *Evaluation of the QUIC Pressure Solver using wind-tunnel data from single and multi-building experiments*. 6th AMS Symp. Urban Environment, Atlanta, GA, LA-UR-05-9016, 12 pp.

2.3 Other Building Pressure Studies

Summary: several non-LANL researchers have applied QUIC to pressure-on-buildings applications. Although they do not include comparisons to experimental data, they do show the importance of building pressure calculations on the amount of natural ventilation (leakiness) and subsequent indoor concentrations.

Sources:

Ashraf, A.M., Argyropoulos, C.D., Olewski, T., Vechot, L. and Kakosimos, K., 2016. *Comparative study on toxic gas infiltration in a non-process area using CFD and multi-zone models*. Symp. Series No. 161, Hazards 26.

Bieringer, P.E., Longmore, S., Bieberbach, G., Rodriguez, L.M., Copeland, J. and Hannan, J., 2013. *A method for targeting air samplers for facility monitoring in an urban environment*. Atmospheric Environment, 80, 1-12.

Herring, S.J., Batchelor, S., Bieringer, P.E., Lingard, B., Lorenzetti, D.M., Parker, S.T., Rodriguez, L., Sohn, M.D., Steinhoff, D. and Wolski, M., 2016. *Providing pressure inputs to multizone building models*. Building and Environment, 101, pp.32-44.

3. QUIC-URB Wind Solver

The wind fields produced by the fast-running empirical-diagnostic wind solver QUIC-URB have been evaluated against wind measurements from wind-tunnel experiments around individual buildings and groups of buildings, as well as from outdoor field experiments. A description of the wind solver equations and solution methods can be found in:

Pardyjak, E.R. and M. Brown, 2003. *QUIC-URB v. 1.1: Theory and User's Guide*, LA-UR-07-3181, 22 pp.

Nelson, M., B. Addepalli, F. Hornsby, A. Gowardhan, E. Pardyjak, and M. Brown, 2008: *Improvements to a fast-response urban wind model*, 15th AMS/AWMA Met. Aspects Air Poll., LA-UR-08-0206, 6 pp.

Brown, M., A. Gowardhan, M. Nelson, M. Williams, E. Pardyjak, 2013. *QUIC transport and dispersion modelling of two releases from the Joint Urban 2003 field experiment*, Int. J. Env. Poll., 52 (3-4) 263-287.

3.1 Buildings

3.1.1 Oklahoma City Joint Urban 2003

Neophytou M., A. Gowardhan, & M. Brown, 2011: *An inter-comparison of three urban wind models using the Oklahoma City Joint Urban 2003 wind field measurements*. Int. J. Wind Eng. & Indust. Aero., 99(4) 357-368.

Summary: a comparison of the QUIC-URB, QUIC-CFD, and QUIC-LES wind solvers to the street-level wind measurements obtained in downtown Oklahoma City during the Joint Urban 2003 Field Experiment. Statistically, the CFD and LES codes performed slightly better than the fast-running QUIC-URB wind solver (however, in other analyses, the comparison to tracer data was statistically similar when using the QUIC-URB wind solver as compared to QUIC-CFD).

Example results:

Table 2

Calculated percentage error for each model in each IOP case, for wind speed and wind direction; the symbols OBS and SIM represent the observed and simulated/predicted values, respectively.

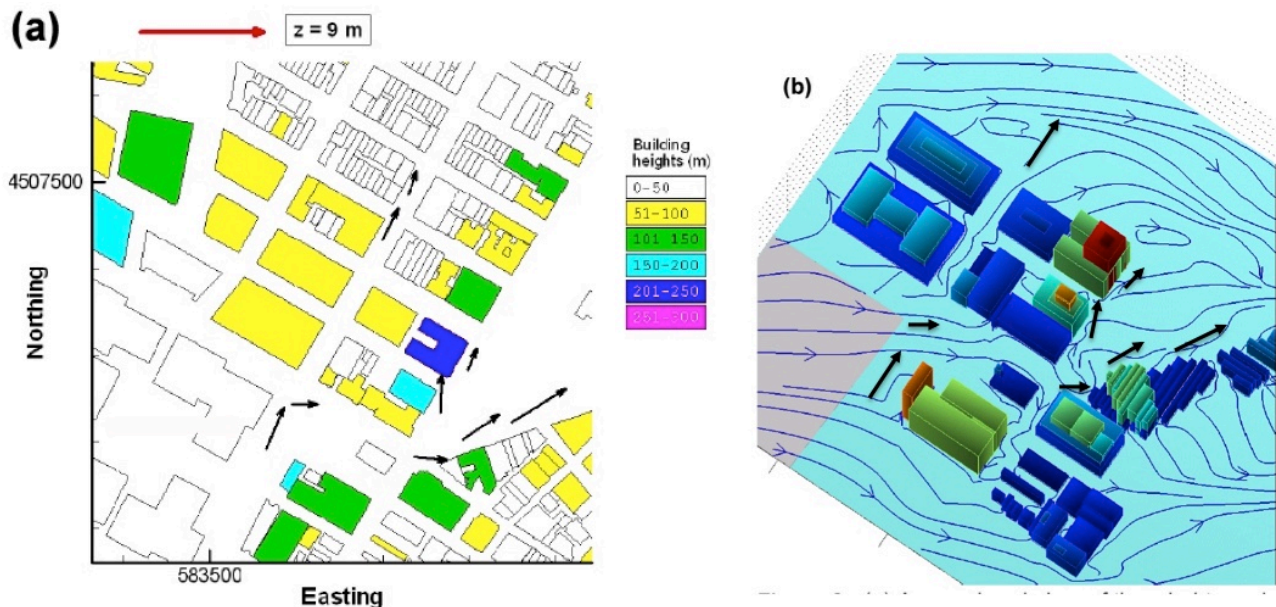
	Wind speed error, $Error = \frac{ OBS-SIM }{0.5 \times (OBS+SIM)}$				Wind direction error, $Error = OBS-SIM $			
	<=100%	<=50%	<=25%	<=10%	<=90°	<=45°	<=30°	<=15°
IOP 2								
Q-URB	71%	47%	27%	14%	77%	65%	48%	32%
Q-CFD	88%	71%	37%	14%	84%	75%	63%	38%
Q-LES	82%	41%	27%	10%	77%	68%	57%	38%
IOP 8								
Q-URB	85%	51%	35%	13%	77%	52%	43%	30%
Q-CFD	85%	58%	33%	16%	86%	59%	54%	38%
Q-LES	87%	60%	18%	5%	77%	68%	57%	38%
IOP 9								
Q-URB	79%	48%	23%	4%	77%	57%	39%	20%
Q-CFD	90%	57%	30%	13%	91%	68%	57%	41%
Q-LES	84%	57%	43%	23%	91%	70%	50%	34%

3.1.2 NYC Lower Manhattan Wind-Tunnel Experiment

Bowker, G., S. Perry, and D. Heist, 2004: A comparison of airflow patterns from the QUIC model and an atmospheric wind tunnel for a two-dimensional building array and multi-block region near the World Trade Center site, 5th AMS Urban Env. Conf., Vancouver, B.C., 6 pp.

Summary: In an independent assessment by USEPA researchers “QUIC flow patterns were compared against ... a complex group of buildings surrounding the World Trade Center in lower Manhattan ... QUIC satisfactorily simulated the flow patterns depicting channeling and recirculation patterns within particular street canyons.” Note that only a sub-set of buildings to the east and northeast of WTC rubble pile were included in the QUIC domain.

Example results:



Left: winds measured near street-level in the USEPA wind tunnel. Right: QUIC streamlines with overlay of measured wind vectors (approximated).

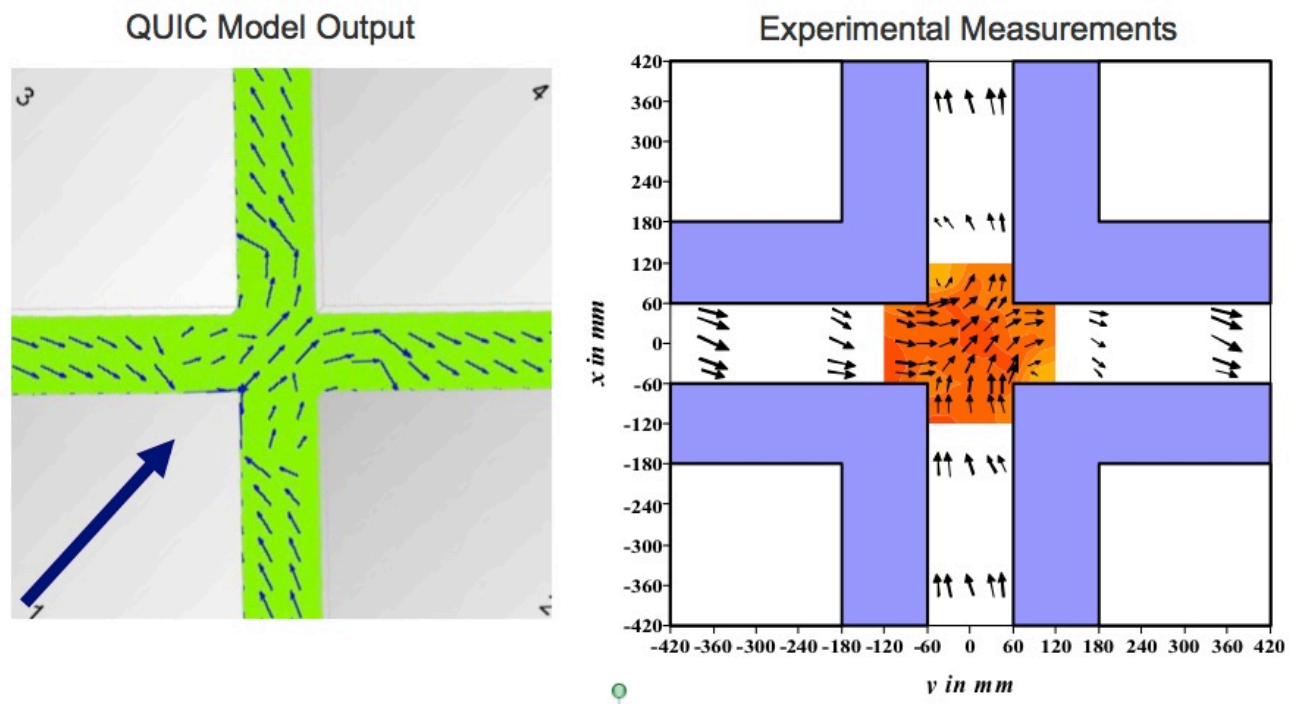
3.1.3 Street Intersection Wind-Tunnel Experiments

Brown, M, 2009: Toxic chemical dispersion modeling in cities and at industrial facilities – evaluation studies, LANL presentation, 42 pp.

Summary: QUIC-URB was compared to intersection flow measurements conducted in the Hamburg wind tunnel by Klein et al. (2007). QUIC was able to fairly reasonably reproduce the flow patterns in the street intersection and the nearby cross streets.

Klein, P., Leidl, B. and Schatzmann, M., 2007. Driving physical mechanisms of flow and dispersion in urban canopies. *International Journal of Climatology*, 27(14), pp.1887-1907.

Example results:



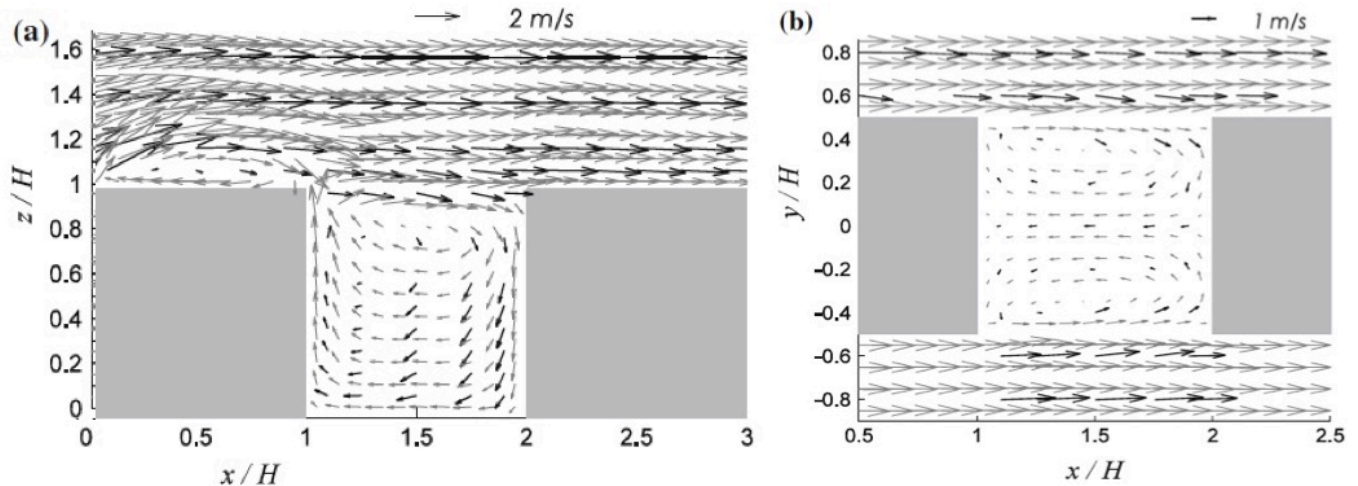
Comparison of (left) QUIC-computed wind fields and (right) measured winds near ground level in a street intersection and nearby cross streets.

3.1.4 Street Canyon Wind-Tunnel Experiments

Singh, B., B. Hansen, M. Brown, E. Pardyjak, 2008: Evaluation of the QUIC-URB fast response urban wind model for a cubical building array and wide building street canyon, *Env. Fluid Mech.*, v 8, pp 281-312.

Summary: A number of studies comparing QUIC-URB wind fields to measurements obtained in street canyons have been performed. In the Singh et al (2008) reference, the wind solver output was compared to wind measurements from a 7x1 wide-building array and a 7x11 cubical-building array. Although there are some key differences, the general circulation pattern and the slowing down of the winds in the street canyon is captured.

Example results:



Comparison of QUIC (gray) and measured (black) wind vectors around cubical building array: a) side view along centerline and b) plan view at building half-height.

Other sources:

Bowker, G., S. Perry, and D. Heist, 2004: *A comparison of airflow patterns from the QUIC model and an atmospheric wind tunnel for a two-dimensional building array and multi-block region near the World Trade Center site*, 5th AMS Urban Env. Conf., Vancouver, B.C., 6 pp.

Gowardhan, A., 2003: *QUIC-URB validation study for 3D cubical building array*, Univ. of Utah Technical Report, 8 pp.

Kastner-Klein, P., E.R. Pardyjak, and M. Brown, 2003: *Evaluation of the fast response model QUIC-URB based on wind-tunnel flow measurements in idealized street canyons*, abstract for the 11th Conf. on Wind Engineering, June 2-5 2003, Lubbock, TX.

Pardyjak, E. and M. Brown, 2002: *Fast response modeling of a two building urban street canyon*, 4th AMS Symp. Urban Env., Norfolk, VA, May 20-24 2002, LA-UR-02-1217.

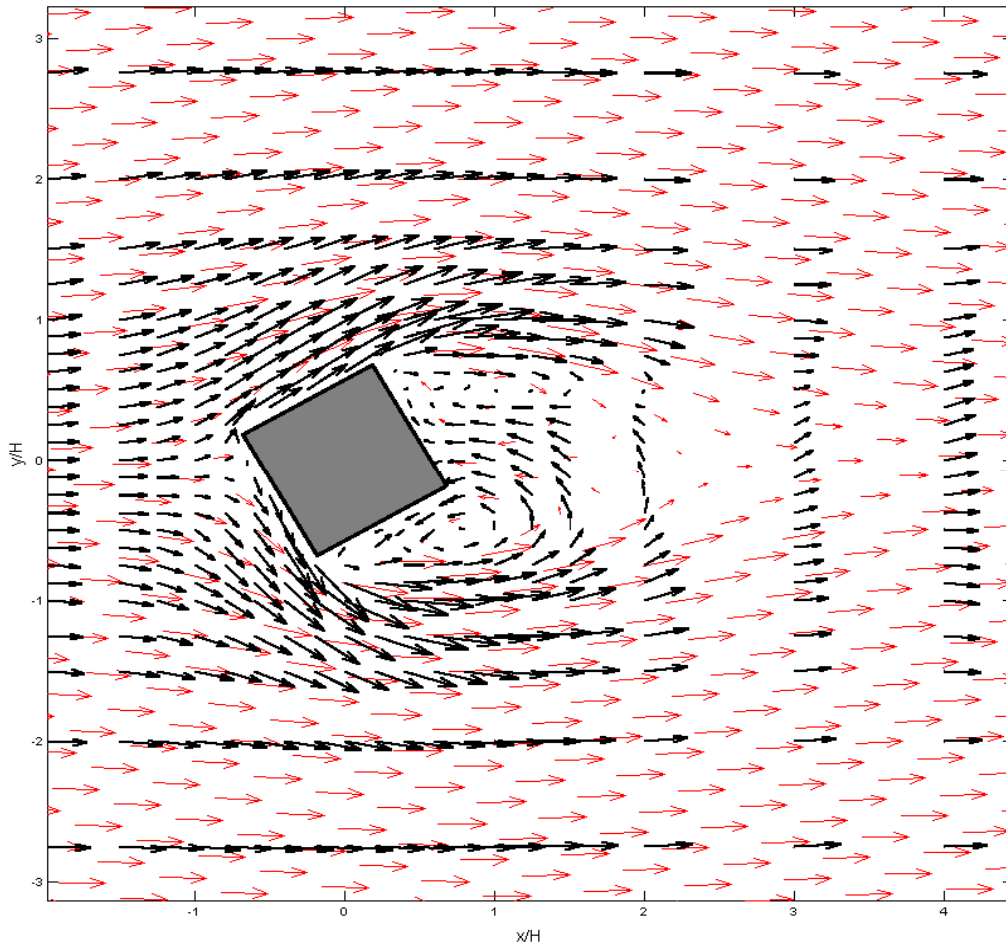
3.1.5 Single-Building Wind-Tunnel Experiments

A large number of studies comparing QUIC-URB wind fields to measurements obtained around isolated buildings have been conducted. Several studies have focused on specific flow features (e.g., the upwind recirculation zone, the rooftop recirculation zone, the downwind cavity), others on different sizes and shapes of buildings, and others at the impact of wind direction on the building recirculation patterns.

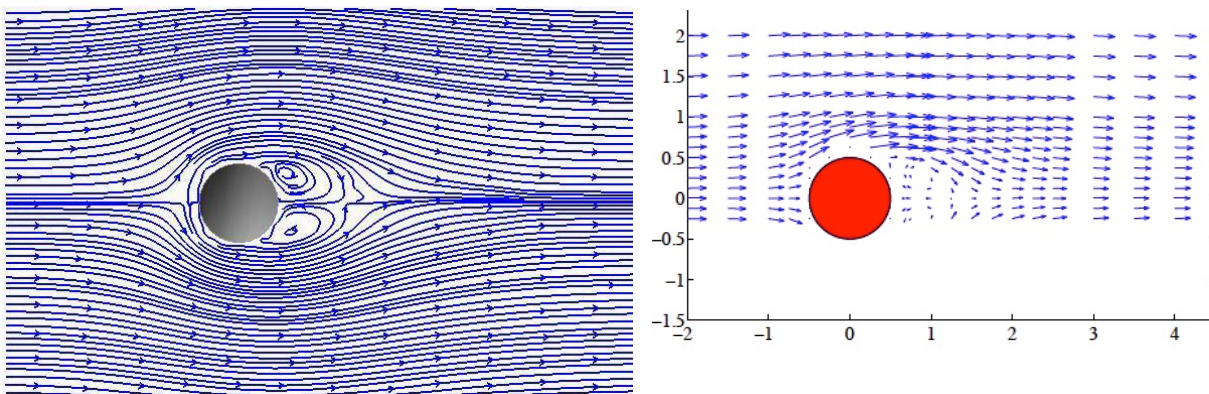
Nelson, M., B. Addepalli, F. Hornsby, A. Gowardhan, E. Pardyjak, and M. Brown, 2008: *Improvements to a fast-response urban wind model*, 15th AMS/AWMA Met. Aspects Air Poll., LA-UR-08-0206, 6 pp.

Summary: Nelson et al. (2008) discusses a number of improvements to the QUIC-URB wind solver, including new algorithms for cylindrical buildings, stadia, and parking garages. The building flow algorithms were modified to work better for flow that hits the building at an oblique angle (i.e., not perpendicular to the front face). The original algorithms overestimated the length of the downwind cavity. The new algorithms do a much better job of approximating the size of the cavity, although there are still some differences in wind directions at specific locations within the cavity zone.

Example results:



Plan-view comparison of QUIC (red) and measured (black) wind vectors around cubical building for inflow wind at 30 deg. relative to the building front face.



Plan view of (left) QUIC-URB computed streamlines around cylinder and (right) PIV measurements from Kappler (2002).

Pol S., N. Bagal, B. Singh, M. Brown, and E. Pardyjak, 2006: *Implementation of a rooftop recirculation parameterization into the QUIC fast response wind model*, 6th AMS Urb. Env. Symp., Atlanta, GA, LA-UR-05-8631, 19 pp.

Summary: In this study, Pol et al. (2006) developed a better rooftop algorithm for the QUIC-URB wind solver to better capture 1) the size and shape of the vortex and strength of the reverse flow that develops on the rooftop for perpendicular flow and 2) the delta-wing vortex that develops under oblique angle flow. The model output was compared to wind measurements for a variety of building heights, widths, and lengths. Although the rooftop measurements were sparse, the shape and size of the vortex matched the measurements fairly well.

Example results:

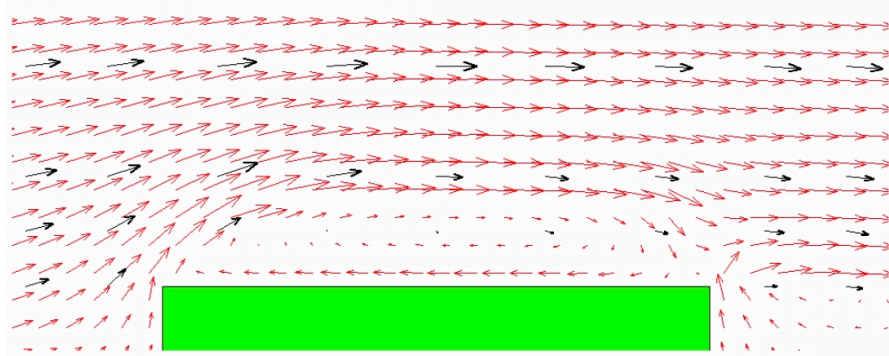
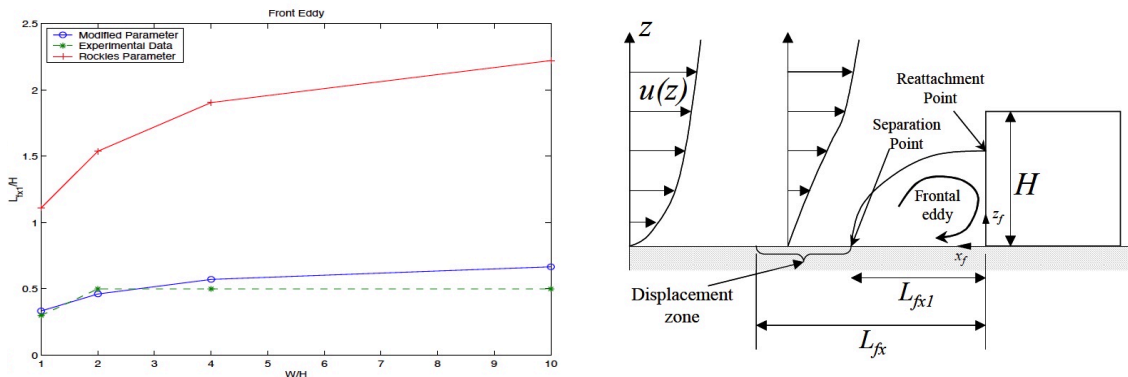


Figure 3: Velocity vector plot with experimental data (\rightarrow) and model computed with new roof top recirculation scheme (\rightarrow) for a cubical building ($W=H=L$) along the center plane for incoming flow perpendicular to the building.

Bagal, N., E. Pardyjak, and M. Brown, 2003: *Improved upwind cavity parameterization for a fast response urban wind model*, AMS Conf. on Urban Zone, Seattle, WA, 3 pp.

Summary: In this study, Pol et al. (2003) developed a better upwind rotor algorithm for the QUIC-URB wind solver to better capture the size and shape of the vortex and strength of the reverse flow that develops on the upwind side of the building. The model-computed length of the upwind recirculation cavity was compared to wind-tunnel measurements for a variety of building width-to-height ratios and agreement was quite good. Comparison to wind measurements made within the rotor were also in reasonable agreement.

Example results:

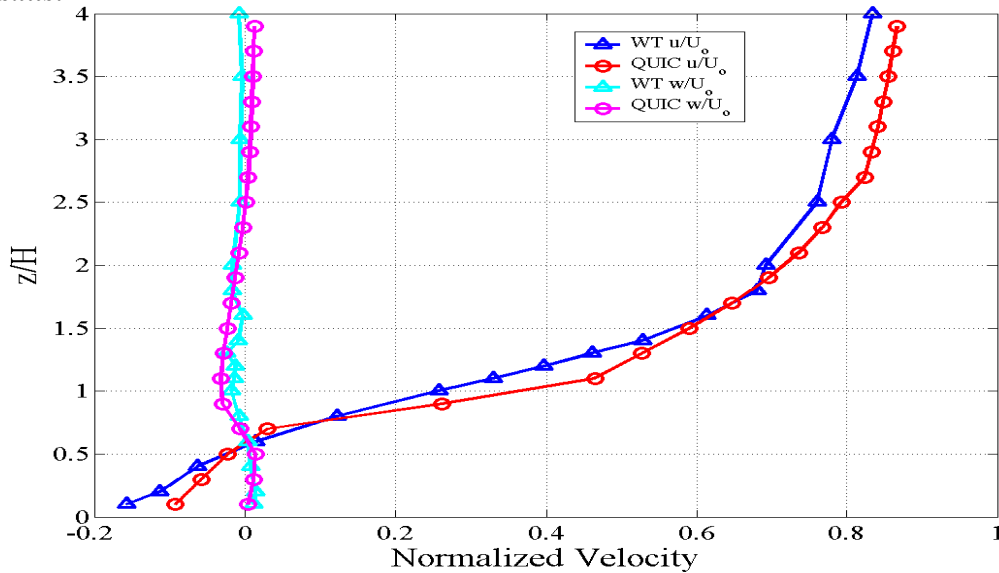


(Left) Comparison of the normalized front eddy length measured in Snyder and Lawson (1994) wind-tunnel experiments to calculations using the original Rockle model (1990) and the new QUIC-URB algorithm for various building width-to-height ratios. (Right) Illustration of the upwind boundary-layer flow near a rectangular obstacle.

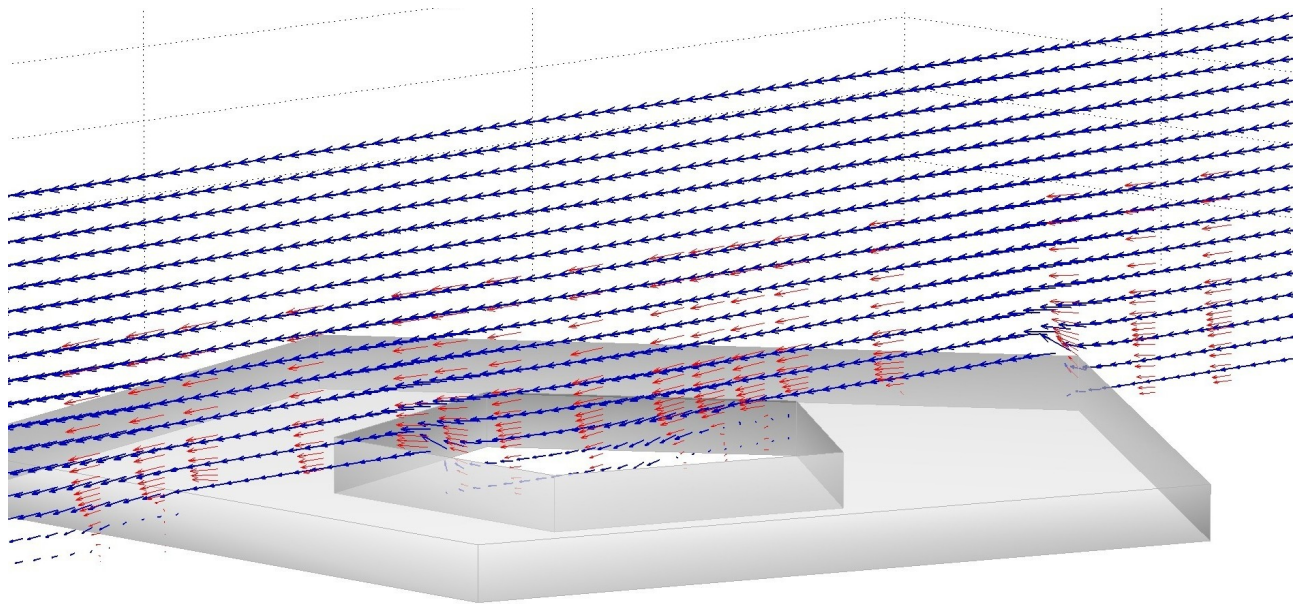
Nelson, M., M. Brown, M. Williams, 2006: *Integration of the Pentagon building into the QUIC dispersion modeling system and testing against wind-tunnel data*, LA-CP-06-0360, 59 pp.

Summary: Nelson et al. (2006) describes the USEPA wind tunnel experiments conducted around a reduced-scale Pentagon building. The QUIC-URB building flow algorithms developed specifically for the Pentagon are described and comparisons to experimental wind measurements show fairly good agreement.

Example results:



Comparison of QUIC-URB computed and measured vertical profiles of horizontal (u) and vertical velocity (w) located near the center of the Pentagon courtyard for a 208° inflow wind direction.



Comparison of the centerline velocity vectors for point impinging flow regime from the wind tunnel data (red) and the QUIC model (blue).

Other sources:

Bagal, N., E. Pardyjak, and M. Brown, 2004: *Implementation of a rooftop recirculation parameterization into the QUIC fast response urban wind model*, 5th AMS Urban Env. Conf., Vancouver, B.C., LA-UR-04-5132, 7 pp.

Pardyjak, E.R., N. L. Bagal and M. J. Brown, 2003: *Improved velocity deficit parameterizations for a fast response urban wind model*, AMS Conf. on Urban Zone, Seattle, WA, LA-UR-03-8512.

Pardyjak, E. and M. Brown, 2001: *Evaluation of a fast-response urban wind model – comparison to single-building wind-tunnel data*, Int. Soc. Environ. Hydraulics, Tempe, AZ, Dec. 2001, LA-UR-01-4028, 6 pp.

Singh, B., E. Pardyjak, and M. Brown, 2004: *Testing of a Far-wake Parameterization for a Fast Response Urban Wind Model*, 6th AMS Urban Env. Conf., Atlanta, GA, 11 pp.

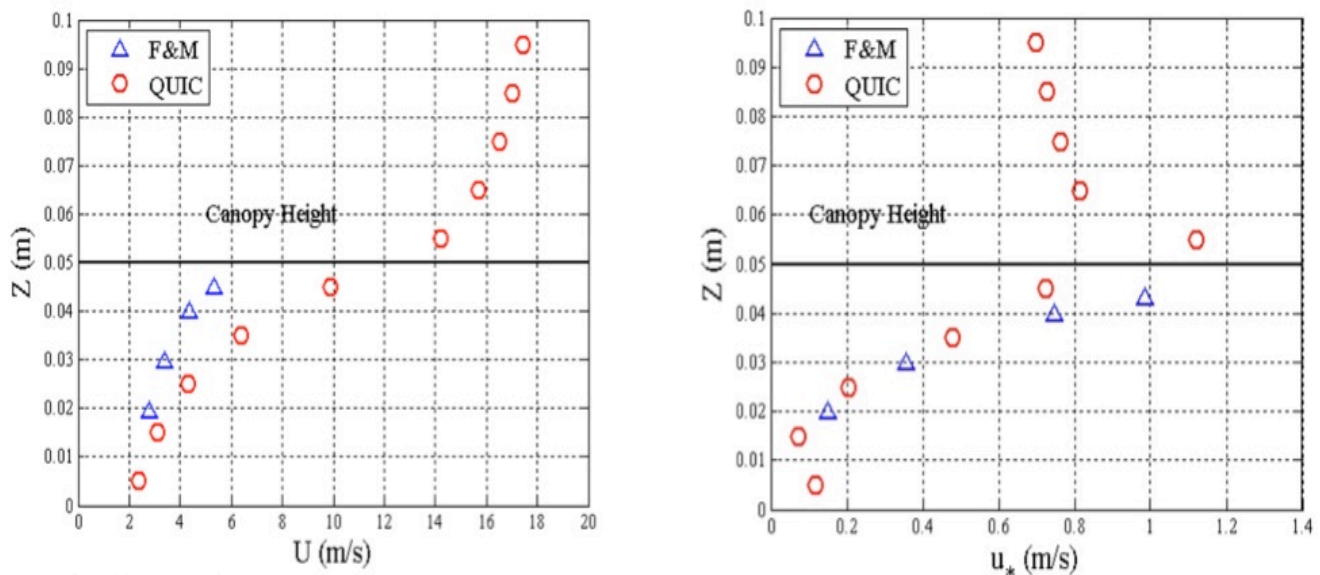
Warner, T.T., P. Benda, S. Swerdlin, J. Knievel, E. Argenta, B. Aronian, B. Balsley, J. Bowers, R. Carter, P. Clark, K. Clawson, J. Copeland, A. Crook, R. Frehlich, M. Jensen, Y. Liu, S. Mayor, Y. Meillier, B. Morley, R. Sharman, 2007: *The Pentagon Shield field experiment: toward protecting national assets*. *Bulletin of the American Meteorological Society*, 88, 167-176.

3.2 Tree Canopies

Nelson, M.A., M. D. Williams, D. Zajic, E. R. Pardyjak, and M. J. Brown, 2009: *Evaluation of an Urban Vegetative Canopy Scheme and Impact on Plume Dispersion*, AMS 8th Symp. Urban Env., Phoenix AZ.

Summary: Nelson et al. (2009) evaluated the vegetative canopy scheme in QUIC against wind-tunnel experiment data of Finnigan and Mulhearn (1978). The comparison showed that the QUIC-URB winds were dramatically slower below canopy height, but the wind measurements showed even more reduction, especially near the canopy top. The QUIC forest canopy turbulence scheme (part of QUIC-PLUME) produced a local friction velocity u^* that matched the measurements fairly well.

Example results:

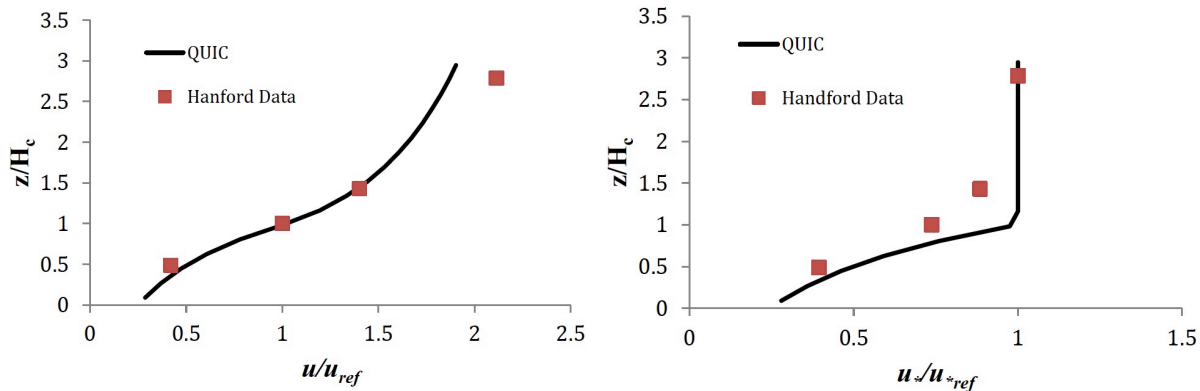


Comparison of QUIC-computed and measured (left) wind speed and (right) friction velocity u^* as a function of height in a plant canopy showing the characteristic slow down of the winds due to plant canopy drag effects.

Pardyjak, E., Veranth, J., Speckart, S., Moran, S. and Price, T., 2013: *Development of a Windbreak Dust Predictive Model and Mitigation Planning Tool*, 73 pp, SERDP RC-1730 Final Report, DTIC ADA602245.

Summary: As part of study on wind breaks and particle deposition, Pardyjak et al. (2013) evaluated the vegetative canopy scheme in QUIC against field experiment data collected in a semi-arid brush canopy region of Hanford, WA. The QUIC-URB produced normalized wind speed and local friction velocity profiles within and slightly above the canopy matched the data fairly well.

Example results:

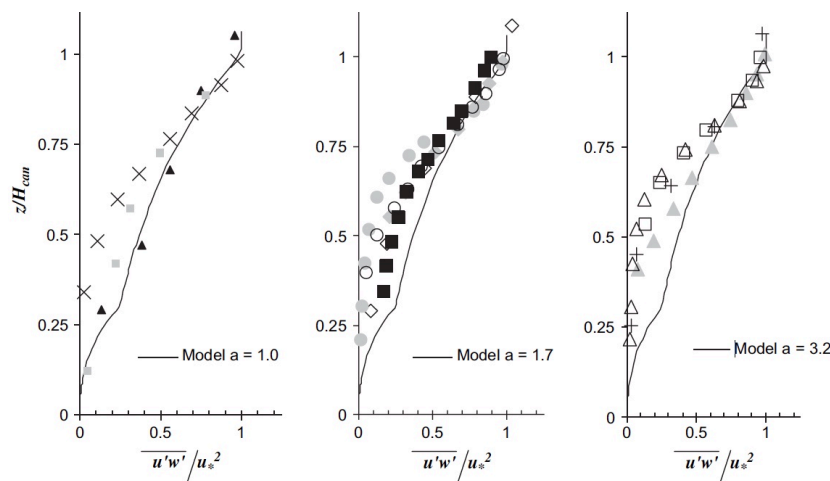


Comparison of QUIC-computed and field measurements of (left) normalized wind speed and (right) normalized friction velocity u_ as a function of height in a scrubland plant canopy in Hanford, Washington.*

Pardyjak, E.R., Speckart, S., Yin, F., Veranth, J.M., 2008. *Near source deposition of vehicle generated fugitive dust on vegetation and buildings: model development and theory*. *Atmos. Environ.*, 42, 6442-6452.

Summary: Pardyjak et al. (2008) evaluated the QUIC-computed Reynolds shear stress ($u_*'^2$) as a function of height against a broad range of wind tunnel and field canopy experiments and showed reasonable agreement but with a fairly consistent slight model over prediction in the lower half of the canopy.

Example results:



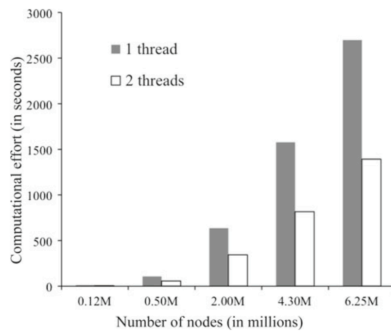
Comparison of QUIC-computed and measured normalized Reynolds shear stress for (left) low, (center) medium, and (right) high density canopies. The variable “a” is the canopy attenuation coefficient.

Other sources:

Booth, T., 2003: *Testing and implementation of urban and plant canopy parameterizations into the Quick Urban & Industrial Complex (QUIC) dispersion modeling system*, Univ. of Utah Technical Report, 8 pp.

4. QUIC-CFD Wind Solver

The wind fields produced by the computational fluid dynamics wind solver QUIC-CFD have been evaluated against wind measurements from wind-tunnel experiments around individual buildings and groups of buildings, as well as from outdoor field experiments. Run times are slower than QUIC-URB (see figure below), but because QUIC-CFD is solving both the mass and momentum conservation equations it is expected to provide a better flow field solution.



A description of the QUIC-CFD equations and solution methods can be found in:

Gowardhan, A., E. Pardyjak, I. Senocak, and M. Brown, 2011: A CFD-based wind solver for an urban fast response transport and dispersion model, *Env. Fluid Mech.*, v 11, iss. 5, p. 439-464.

Gowardhan, A., 2008: Towards understanding complex flow phenomenon in urban areas using numerical tools, Ph.D. dissertation, University of Utah, UT.

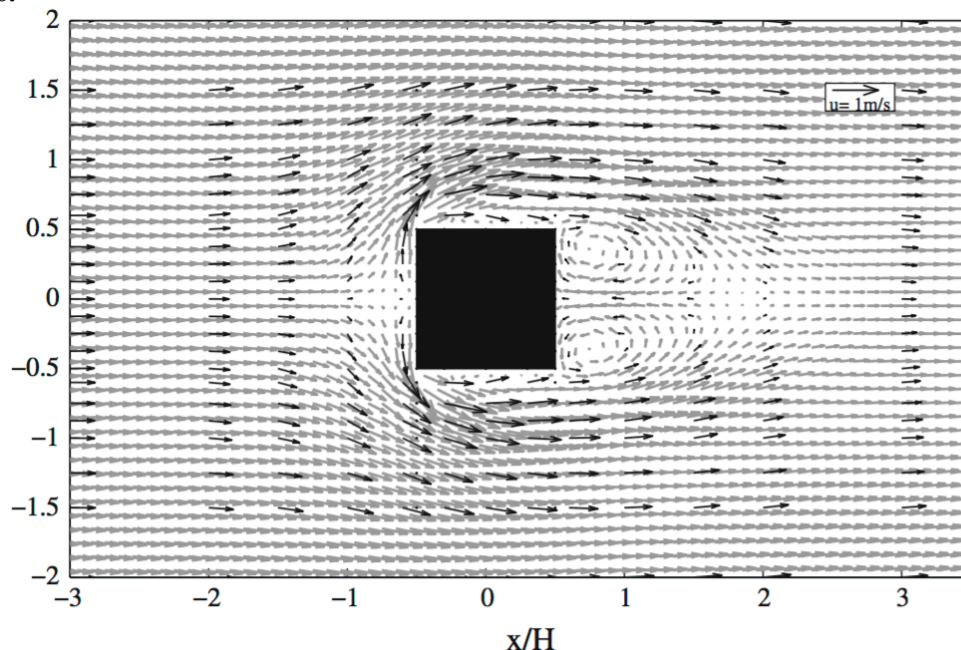
4.1 Wind-Tunnel Experiments

4.1.1 Cubical Building

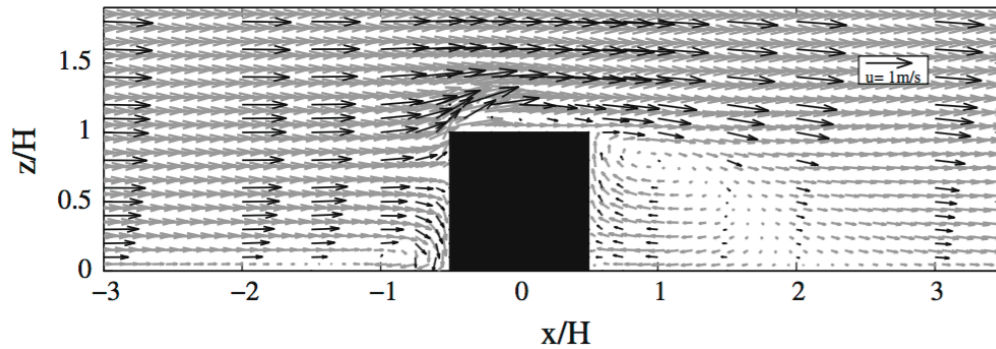
Gowardhan, A., E. Pardyjak, I. Senocak, and M. Brown, 2011: A CFD-based wind solver for an urban fast response transport and dispersion model, *Env. Fluid Mech.*, v 11, iss. 5, p. 439-464.

Summary: QUIC-CFD was evaluated against an isolated cube wind tunnel experiment conducted at the USEPA Fluid Modeling Facility. Major flow circulation features in front of and behind the cube were well approximated by the QUIC-CFD flow solver, except for the rooftop recirculation bubble.

Example results:



Comparison of QUIC-computed and measured wind vectors on a near-surface horizontal plane at $z/H = 0.1$.
Gray vectors: QUIC-CFD and Black vectors: measurements.



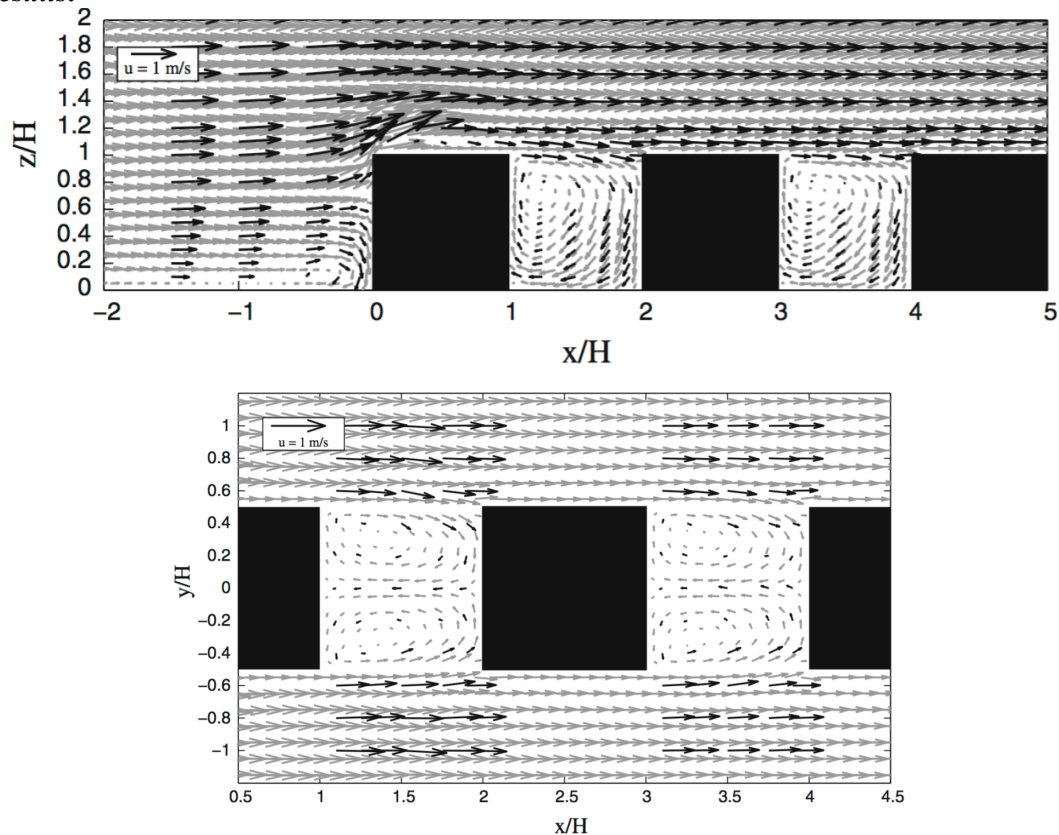
Comparison of QUIC-computed and measured wind vectors on the centerline x - z vertical plane.
Gray vectors: QUIC-CFD and Black vectors: measurements.

4.1.2 Idealized Building Array

Gowardhan, A., E. Pardyjak, I. Senocak, and M. Brown, 2011: A CFD-based wind solver for an urban fast response transport and dispersion model, *Env. Fluid Mech.*, v 11, iss. 5, p. 439-464.

Summary: QUIC-CFD was evaluated against wind measurements from a 7x11 array of cubes in a wind tunnel experiment conducted at the USEPA Fluid Modeling Facility. The QUIC-CFD code was able to simulate the major circulation features between and around the buildings. The rooftop recirculation zone on the front-most building was not captured, however, at the given vertical grid resolution.

Example results:



Comparison of QUIC-computed and measured wind vectors (top) on the centerline x - z plane and (bottom) on a near-surface horizontal plane at $z/H = 0.1$. Gray vectors: QUIC-CFD and Black vectors: measurements.

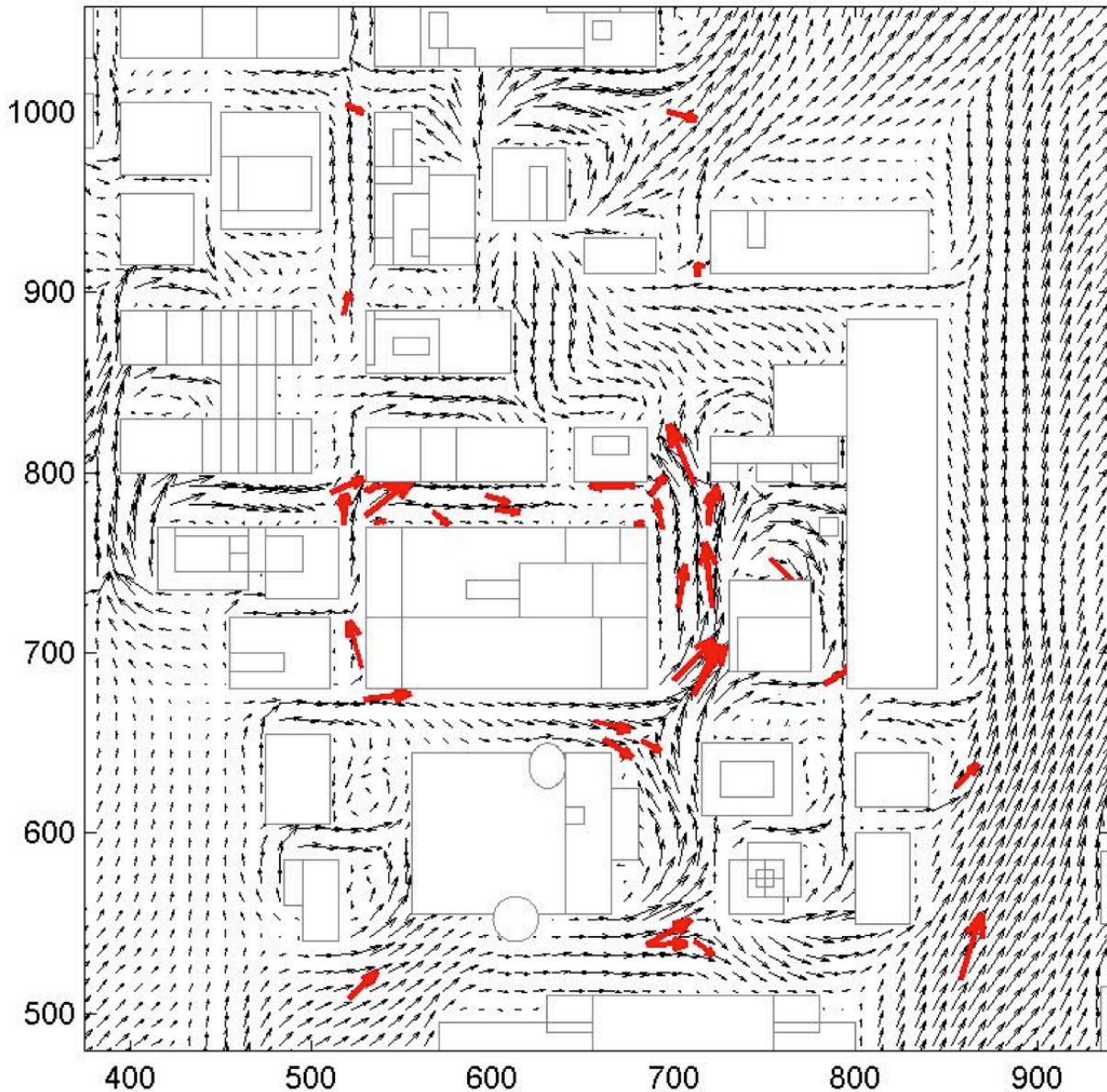
4.2 Outdoor Field Experiments

4.2.1 Oklahoma City Joint Urban 2003

Neophytou M., A. Gowardhan, & M. Brown, 2011: An inter-comparison of three urban wind models using the Oklahoma City Joint Urban 2003 wind field measurements. Int. J. Wind Eng. & Indust. Aero., 99(4) 357-368.

Summary: a comparison of the QUIC-URB, QUIC-CFD, and QUIC-LES wind solvers to the street-level wind measurements obtained in downtown Oklahoma City during the Joint Urban 2003 Field Experiment. Statistically, the CFD and LES codes performed slightly better than the fast-running QUIC-URB wind solver.

Example results:



Comparison of the measured 30-min averaged street-level winds (red) and the computed QUIC-CFD wind field in downtown Oklahoma City (IOP 2, Release 1, 10:00-10:30 CST, July 2, 2003).

5. QUIC-PLUME Transport and Dispersion Model

Different aspects of the QUIC-PLUME random-walk plume model have been evaluated against numerous field, wind tunnel, and laboratory experiments. The QUIC-PLUME transport and dispersion model has been validated for cases over flat terrain and around buildings, as well as for neutral, dense, and buoyant releases. Specific algorithms within QUIC-PLUME have been evaluated against controlled laboratory experiments focusing on phenomenon such as gravitational settling, droplet evaporation, liquid pool growth, surface deposition, and secondary evaporation. A detailed description of the QUIC-PLUME random-walk equations, turbulence schemes, and various specialized source term and transport and dispersion algorithms can be found in:

Williams, M., M. Brown, M. Nelson, 2009: QUIC-PLUME Theory Guide, 41 pp.

5.1 Flat Terrain Neutrally-Buoyant Tracer Experiments and Tests

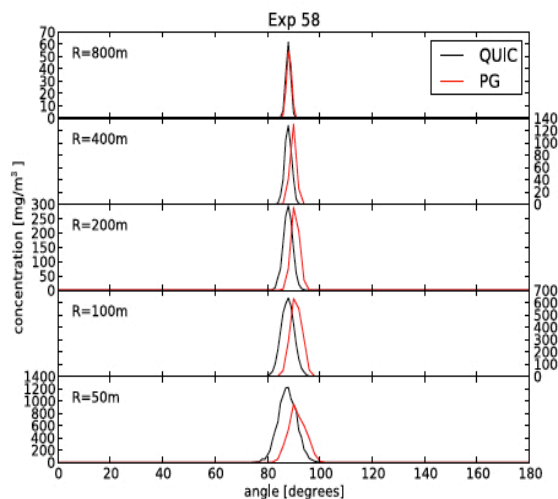
In order to ensure that the QUIC-PLUME random-walk transport and dispersion solver is properly accounting for turbulent mixing under different wind and atmospheric stability conditions, the code has been evaluated against neutrally-buoyant tracer experiments conducted in flat terrain, as well as compared to the solutions from flat-earth Gaussian and non-Gaussian plume models.

5.1.1 Project Prairie Grass Point Source Tracer Field Experiment

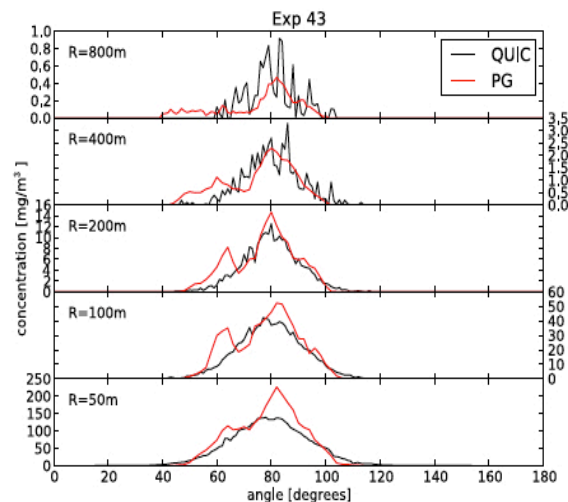
Heagy, J. and Fregeau, J., 2011. Military protective action distances (MPAD): A pilot study. 15th GMU Conf. Atm. T&D Modeling, Fairfax, VA.

Summary: Using the classic flat-earth point-source transport and dispersion experiment Project Prairie Grass, Heagy and Fregeau (2011) independently evaluated QUIC-PLUME using surface concentration samplers on arcs at five different distances from the. They found fairly good agreement between the measured and model-computed lateral plume spread for stable, neutral and unstable conditions.

Example results:



**Excellent overall agreement;
QUIC slightly overpredicts PG at short range.**



**Good overall agreement;
QUIC appears to underpredict PG at long range**

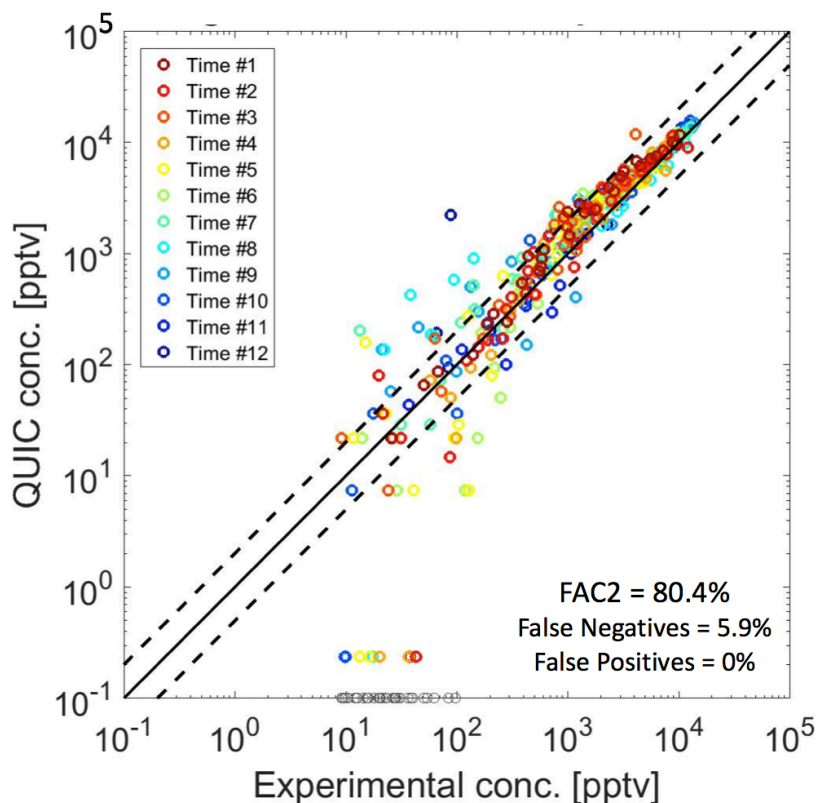
Comparison of QUIC-computed lateral concentration profiles compared to Project Prairie Grass measurements on arcs at five different downwind distances from a point source release: (left) nighttime stable conditions and (right) daytime unstable conditions.

5.1.2 Idaho National Laboratory Line Source Field Experiments

Brambilla, S. and M. Brown, 2017. LANL Internal Study. Journal article in preparation.

Summary: QUIC-PLUME was evaluated using tracer measurements downwind of SF₆ line source releases over flat scrubland terrain conducted at Idaho National Laboratory (see Finn et al. (2010) "Tracer studies to characterize the effects of roadside noise barriers on near-road pollutant dispersion under varying atmospheric stability conditions"). The nearest downwind measurements were within 18 m of the line source and six lines of samplers at different downwind distances extended out to 180 m downwind. For a series of twelve near-neutral stability strong-wind tracer experiments, the results from QUIC-PLUME were within a factor of two of the measurements just over 80% of the time.

Example results:



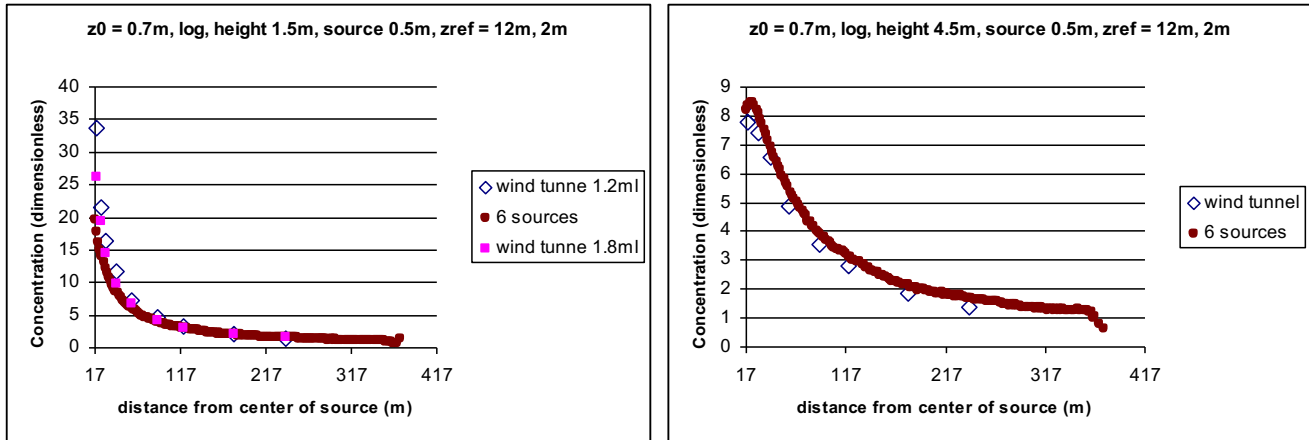
Comparison of QUIC-computed concentrations and measurements downwind of a 54 m line source over flat scrubland terrain for 12 different sets of 15-minute experiments under strong winds and near-neutral stability.

5.1.3 Wind-Tunnel Experiments

Bowker, G., 2004. USEPA Fluid Modeling Facility wind-tunnel experiment. Six line sources over flat surface. Personal Communication.

Summary: As part of a sound-barrier wind-tunnel plume modeling experiment, Bowker (2004) provided an independent comparison of QUIC-PLUME and concentration measurements at several heights over flat-terrain downwind of six line sources in a neutral turbulent-boundary-layer flow. At tunnel-scale, the nearest concentration measurements were ~0.11 m downwind of the line source. Results were extremely good near the ground with the majority of model-computed values within 30% of the measurements and all within a factor of two.

Example results:



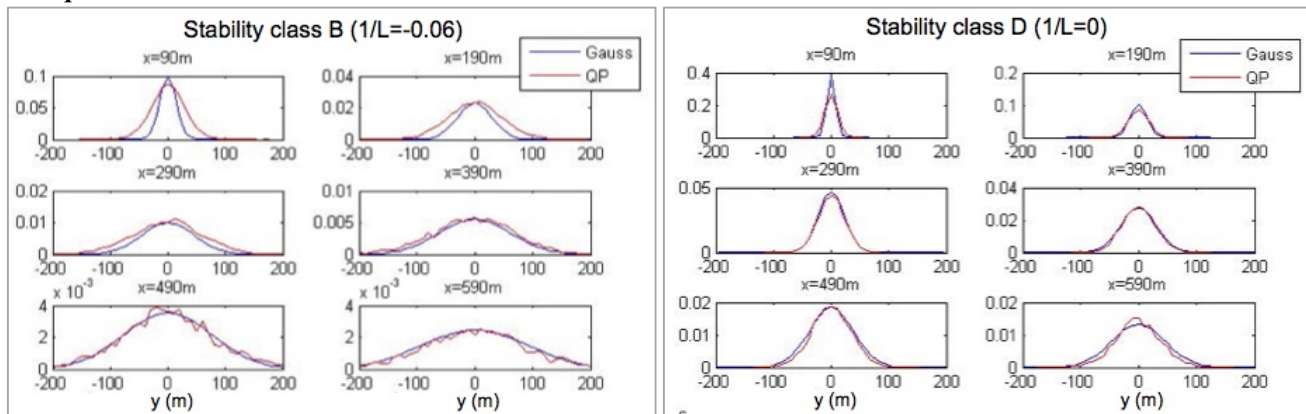
QUIC-computed concentrations at (left) 1.5 m above the ground (agl) and (right) 4.5 m agl compared to concentration measurements downwind of six line-source releases in a flat-terrain wind-tunnel experiment conducted at the USEPA Fluid Modeling Facility (1:150 scale).

5.1.4 Gaussian Plume Model Comparisons

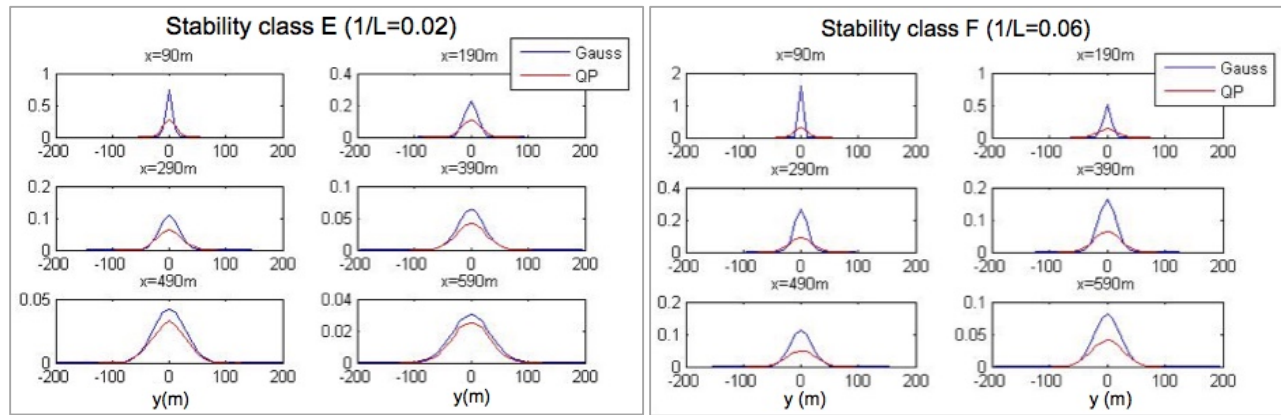
Zajic, D., and Brown, M., 2007. LANL internal testing of QUIC-PLUME stability-dependent routines.

Summary: Zajic and Brown (2007) compared QUIC-PLUME output to Gaussian plume model output as a function of stability. Results show very good agreement for unstable (B) and neutral (D) stability conditions, but for stable conditions the QUIC-PLUME model has lower centerline concentrations when the inverse Obukhov length $1/L = 0.06$ as compared to the Gaussian plume model with stability class E and F. Differences are expected, however, due to the inherent differences in assumptions between the two modeling approaches (e.g., Gaussian: wind speed and turbulence constant with height and discrete stability classes; QUIC-PLUME: wind speed (log-law wind profile) and turbulence varies with height and continuous stability variation based on inverse Obukhov length).

Example results:



Comparison of QUIC-computed lateral concentration profiles and Gaussian plume model output at $z = 2$ m agl at six downwind distances for a point source release under B-unstable and D-neutral stability conditions.

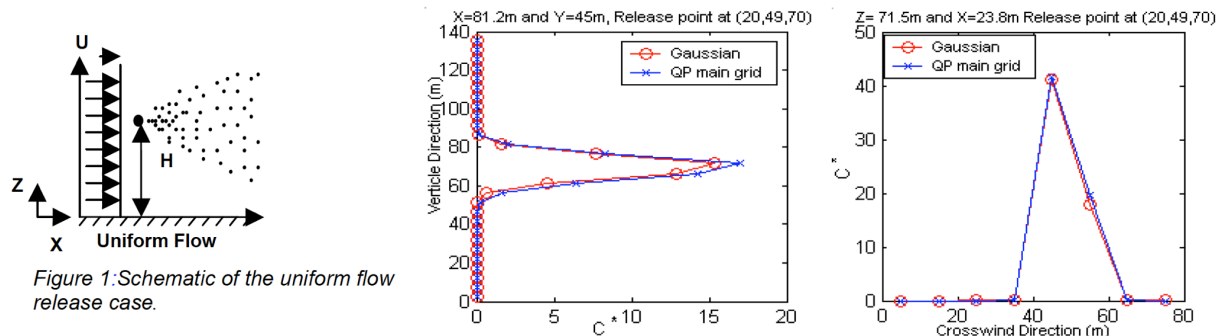


Comparison of QUIC-computed lateral concentration profiles and Gaussian plume model output at $z = 2$ m agl at six downwind distances for a point source release under E-stable and F-stable stability conditions.

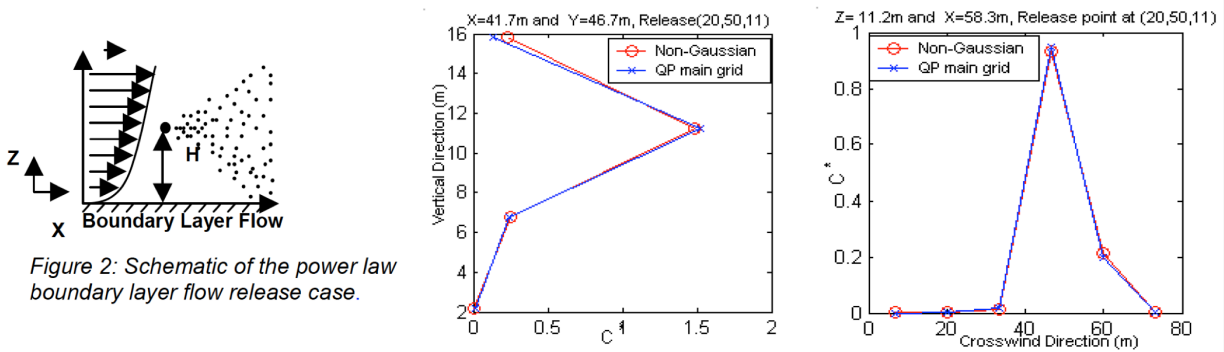
Singh, B., M. Williams, E. Pardyjak, M. Brown, 2003: Validation testing of an urban Lagrangian dispersion model, AMS Conf. on Urban Zone, Seattle, WA, LA-UR-03-8511, 4 pp.

Summary: Singh et al. (2003) compared QUIC-PLUME concentrations to Gaussian (uniform wind) and non-Gaussian (power-law) analytical plume modeling equations for elevated releases in flat terrain under neutral stability. For the uniform wind case, the QUIC-PLUME turbulence algorithms were modified to include an analytically-derived turbulent velocity scale, since the gradient-based turbulence model would produce zero turbulence for a non-physical uniform wind.

Example results:



Comparison of QUIC-computed and Gaussian model-computed concentrations along a (middle) vertical and (right) lateral profile for a uniform wind.



Comparison of QUIC-computed and Gaussian model-computed concentrations along a (middle) vertical and (right) lateral profile for a power-law wind profile.

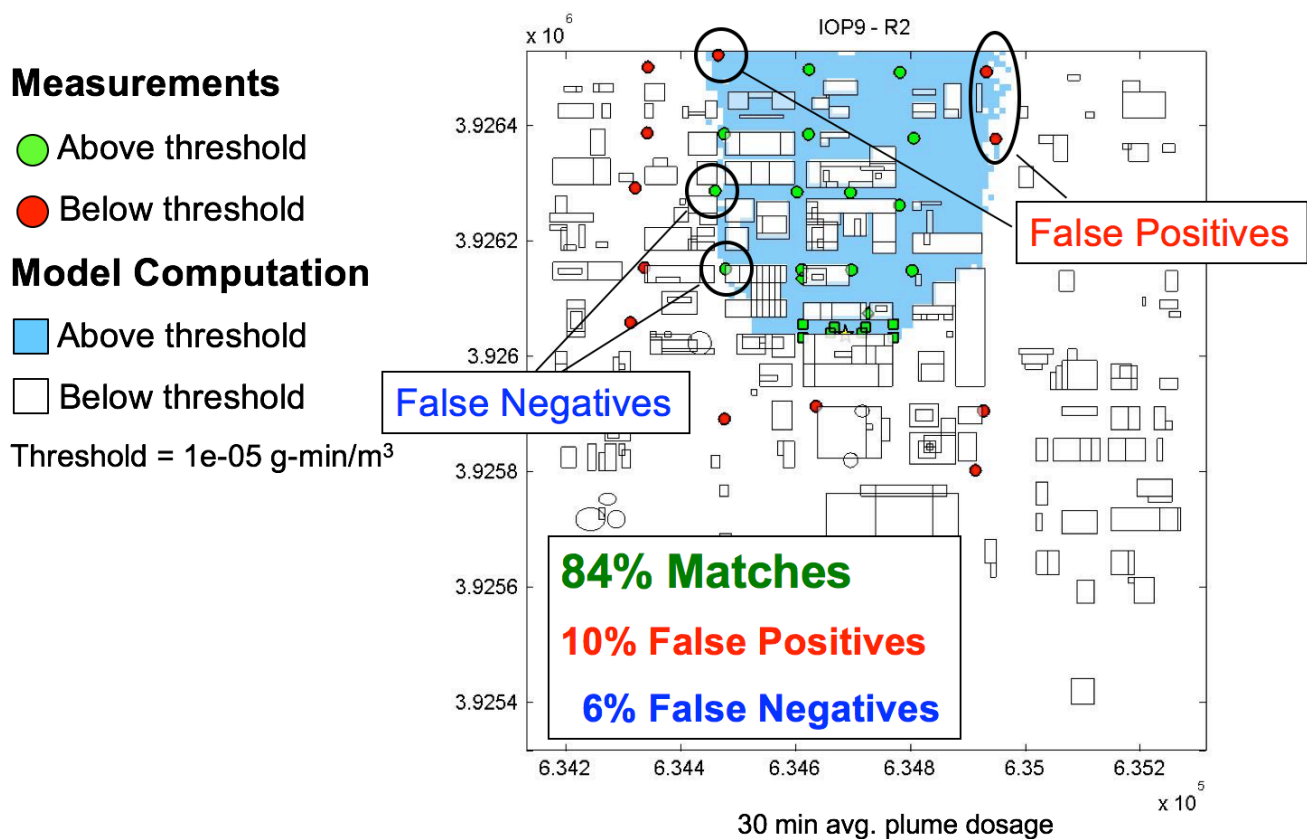
5.2 Urban Tracer Experiments

5.2.1 Oklahoma City Joint Urban 2003

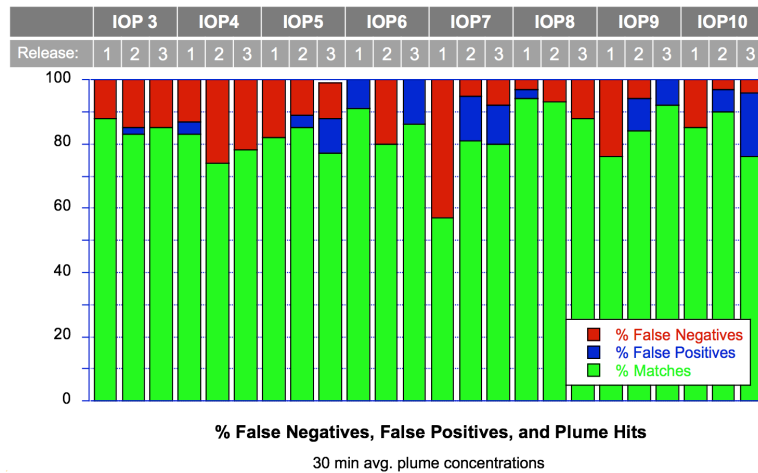
Brown, M., M. Nelson, M. Williams, and S. Brambilla, 2012. *Building-Aware Sensor Siting to Optimize Chemical, Biological, and Radiological Plume Detection*, 17th AMS Conference on Air Pollution Meteorology, presentation.

Summary: The QUIC-URB and QUIC-PLUME models were evaluated against the 30-min duration point-source releases for eight of the ten intensive operating periods (IOPs 3 thru 10) conducted during the Joint Urban 2003 field experiment in downtown Oklahoma City. In this analysis, a threshold dosage was used to compute the percentage of samplers that QUIC correctly predicted to be above the threshold (matches), incorrectly predicted to be above the threshold (false positives), and incorrectly predicted to be below the threshold (false negatives). For the 24 tracer experiments evaluated, QUIC averaged 83% matches, with a high of 94% and an outlier low of 57%. The threshold dosage method of analysis de-emphasizes the point-to-point concentration comparisons and instead highlights whether the broad shape of the plume footprint is correctly matching.

Example results:



Comparison of QUIC-computed 30-minute-average dosages compared to Oklahoma City Joint Urban 2003 measurements using a threshold dosage of $1\text{e-}05 \text{ g-min/m}^3$. For intensive operating period no. 9 and release no. 2 (Park Avenue release), QUIC correctly predicts 84% of the samplers to be above the threshold dosage, while 10% are false positives (i.e., QUIC predicts the sampler is above the threshold, but the sampler measurement is below the threshold) and 6% are false negatives (QUIC is below the threshold, but the measurement is above the threshold).



Barchart of the percentage of QUIC-computed matches, false positives, and false negatives for all the 30-minute-average gas sampler measurements obtained for the 24 point-source releases during IOPs 3 thru 10 of the Oklahoma City Joint Urban 2003 field experiment using a threshold dosage of 1e-05 g-min/m³.

Brown, M.J., Gowardhan, A.A., Nelson, M.A., Williams, M.D. and Pardyjak, E.R., 2013. QUIC transport and dispersion modelling of two releases from the Joint Urban 2003 field experiment. *International Journal of Environment and Pollution*, 52(3-4), pp.263-287.

Summary: The QUIC-URB and QUIC-PLUME models were evaluated against two 30-min duration point-source releases of SF₆ during two intensive operating periods (IOP 2 and IOP 8) conducted during the Joint Urban 2003 field experiment in downtown Oklahoma City. In this analysis, QUIC was compared to every bag surface and rooftop bag samplers, i.e., a paired in time- and space- comparison. The PWID-15 wind sensor located on a tower on a post-office rooftop that was located immediately upwind (to the south) of the OKC central business district was used as input to the model. Plume patterns and extent matched fairly well in all but a few streets. QUIC FAC2 statistics were well above the 30% value proposed by Hanna and Chang (2012) for a successful urban terrain model, even though our statistics were based on all measurements and the more difficult paired-in-space and in-time comparisons and Hanna and Chang were considering the easier arc maximum concentrations only and not paired in space. Comparisons to other CFD codes showed that QUIC was able to do almost as well as or better than these much slower running codes.

Example results:

Joint Urban 2003: IOP2: Release 1

Model	FAC 2	FAC 5	FAC 10	FB	NMSE
Perfect Score	100%	100%	100%	0	0
FEM3MP RANS	NR	63%	NR	-0.76	2.4
QUIC-URB	46%	67%	71%	-0.29	0.6

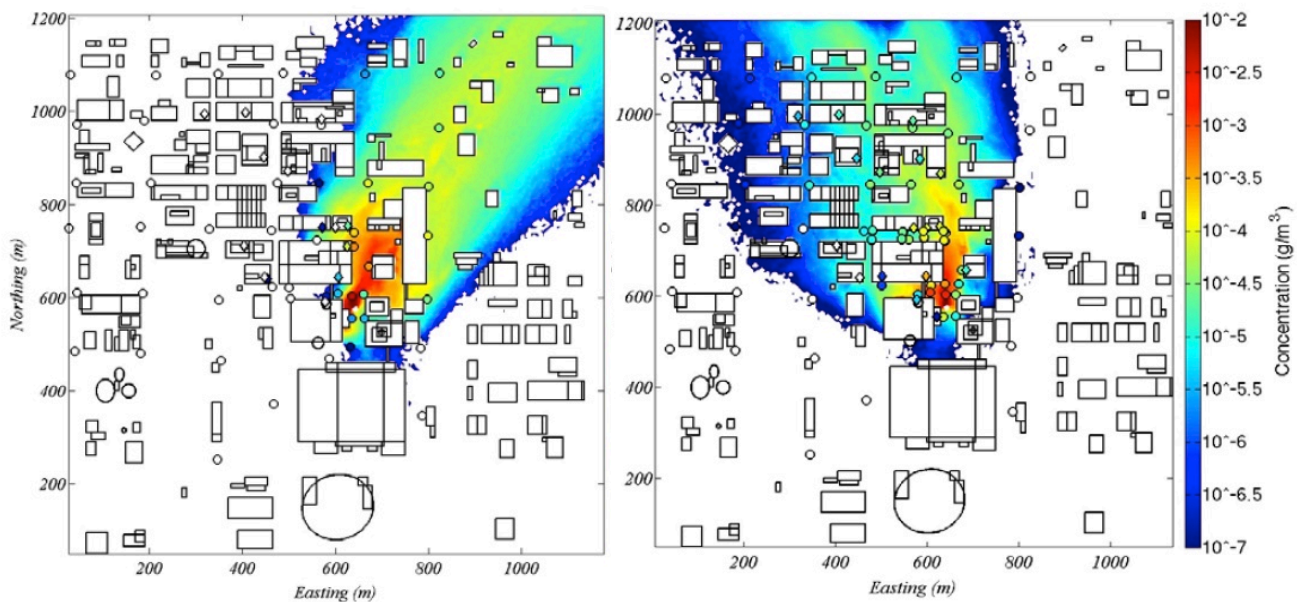
$$FB = 2(\overline{Co} - \overline{Cp}) / (\overline{Co} + \overline{Cp})$$

$$NMSE = ((\overline{Co} - \overline{Cp})^2) / (\overline{Co} \times \overline{Cp})$$

Joint Urban 2003: IOP8: Release 2

Model	FAC 2	FAC 5	FAC 10	FB	NMSE
Aeolus LES	38%	75%	83%	-1.14	28
Aeolus RANS	48%	75%	86%	-0.5	NR
QUIC-URB	45%	73%	81%	-0.74	14.2

Comparison of the fraction of model-computed concentrations that were within a factor of 2, 5, and 10 of the measurements (not including matched zeroes) during the release period compared to full physics (but slower running) computational fluid dynamics codes. FB is fractional bias and NMSE is normalized mean square error.



Comparison of 30-min-averaged model-computed concentrations and measurements during the release period (filled circles) for (left) IOP2, Release 1 (11:00–11:30 am CDT, July 2, 2003) and for (right) IOP8, Release 2 (1:00–1:30 am CDT, July 25, 2003).

Note: The poor model-measurement plume statistics results from the Hanna et al. (2011) paper should not be used to assess the performance of the four different urban plume models evaluated against Joint Urban 2003 field data (one of which is QUIC). The input wind direction to the models was arbitrarily chosen to be a 100 m agl sodar wind, which was later shown to be unrepresentative of the ambient flow during the time period of the release (based on evaluation of many other wind measurement systems). On the other hand, one could use the plume statistics to quantify how a wind direction error of 25 to 30 degrees impact plume transport and dispersion accuracy.

Hanna, S., J. White, J. Troler, R. Vernot, M. Brown, A. Gowardhan, H. Kaplan, Y. Alexander, J. Moussafir, Y. Wang, C. Williamson, J. Hannan, E. Hendrick, 2011: Comparisons of JU2003 observations with four diagnostic urban wind flow and Lagrangian particle dispersion models, *Atmos. Env.*, v 45, iss. 24, p. 4073-4081.

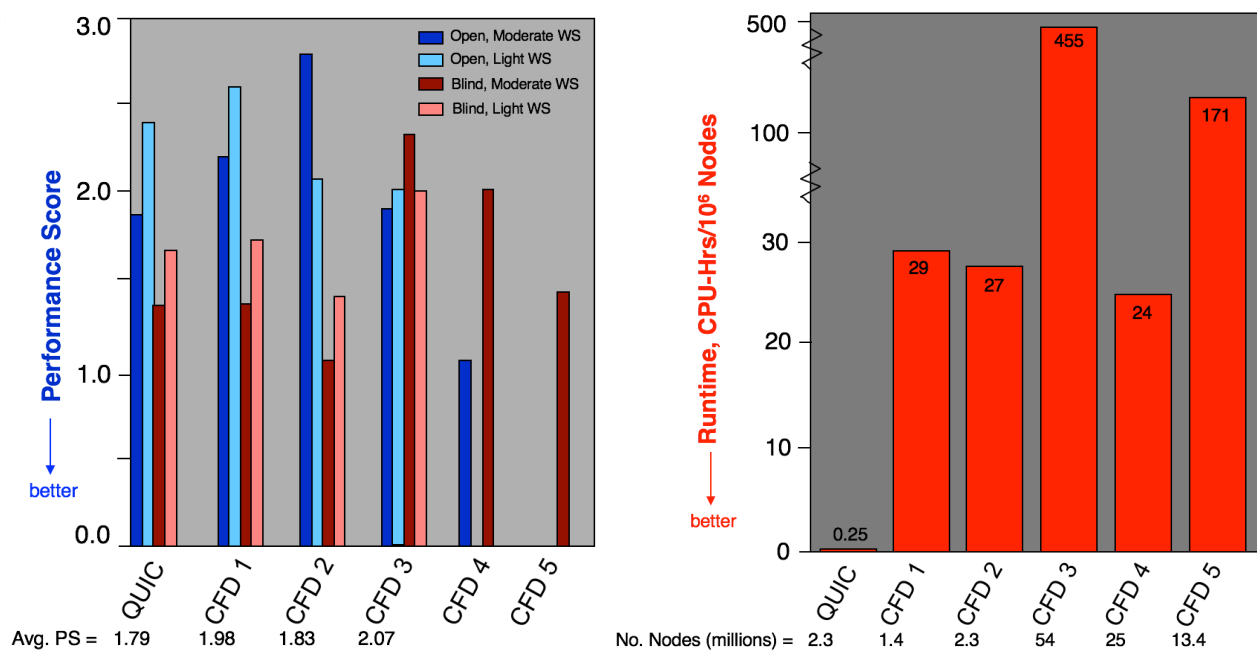
5.2.2 Midtown Manhattan Tracer Experiment

Allwine, K.J., J.E. Flaherty, M. Brown, W. Coirier, O. Hansen, A. Huber, M. Leach, and G. Patnaik, 2008: *Urban Dispersion Program: Evaluation of six building-resolved urban dispersion models*, Official Use Only PNNL-17321 report, 88 pp.

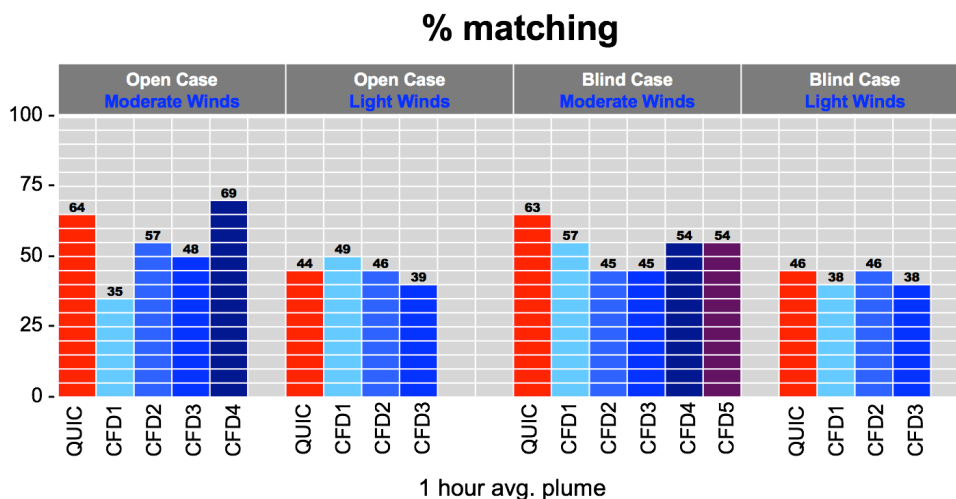
Summary: The QUIC-URB and QUIC-PLUME models were evaluated against 30-min duration PFT and SF6 point-source releases emitted during the Midtown Manhattan field tracer experiment along with five CFD models. Plume model evaluation statistics were independently calculated by PNNL researchers for two 2-hour long experiments in which the modeling teams were allowed to look at the surface-level wind data and tracer measurements (the “Open” cases) and four 2-hour long experiments in which the tracer and street level wind measurements were not shared (the “Blind” cases). Each “Open” case consisted of simultaneous releases of SF6 and a PFT from different locations. For the first “Blind” case, 2 PFT and 1 SF6 release were conducted simultaneously from three different locations, while for the 2nd “Blind” case, 3 PFT’s were releases at 3 different locations. The PNNL team derived a performance score (PS) from six standard metrics (the fraction above a threshold, the fraction within a factor of two, the fractional bias, the geometric mean, the root mean square error, and the geometric root mean square error) and derived it such that PS = 0 is a perfect model. When averaging over all four IOP’s, QUIC had the lowest performance score, but ran hundreds to thousands of times faster than the CFD codes. For the blind cases, QUIC had the 2nd best score out of four models for the light winds IOP and

the 2nd best score out of five models for the moderate winds IOP. In other analyses performed by PNNL, a threshold dosage was used to compute the percentage of samplers that QUIC correctly predicted to be above the threshold (matches), incorrectly predicted to be above the threshold (false positives), and incorrectly predicted to be below the threshold (false negatives). For the 14 tracer experiments evaluated, QUIC averaged 63.5% matches for the moderate wind cases (both blind and open), best among all the models, and 45% matches for the light wind cases within a few percentage points of the CFD models. Note that the threshold dosage method of analysis de-emphasizes the point-to-point concentration comparisons and instead highlights whether the broad shape of the plume footprint is correctly matching.

Example results:



Comparison of (left) the computed performance score (PS = 0 is a perfect model) for QUIC and four other CFD models using the Midtown Manhattan concentration measurements and (right) the run times for the different modeling systems.



Comparison of the percentage of Midtown Manhattan gas samplers correctly predicted by QUIC and CFD models to be above a concentration threshold value (## ppt). The measurements include ## point source releases at # different locations under four different meteorological conditions.

Other sources:

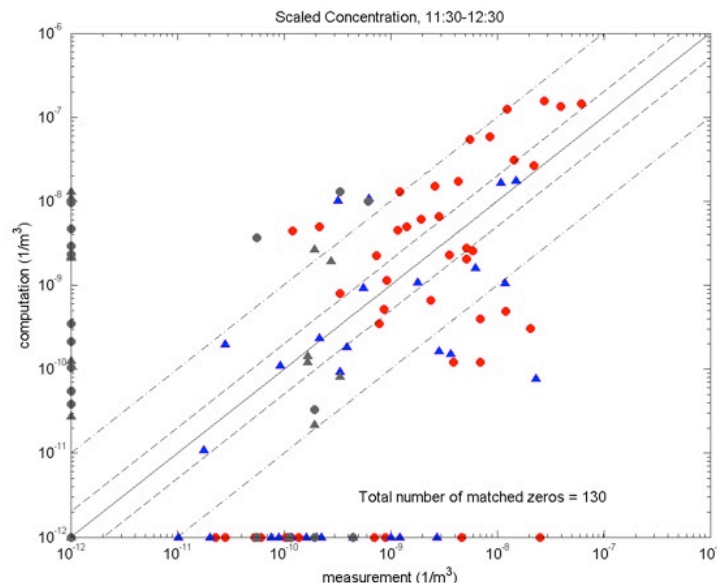
Flaherty, J.E., K.J. Allwine, M.J. Brown, W.J. Coirier, S.C. Ericson, O.R. Hansen, A.H. Huber, S. Kim, M.J. Leach, J.D. Mirocha, R.K. Newsom, and G. Patnaik, I. Senocak, 2007: Evaluation study of building-resolved urban dispersion models, AMS 7th Symp. Urban Env., San Diego, CA, paper 7.2, 4 pp.

5.2.3 Madison Square Garden Tracer Experiment

Senocak, I., A. Gowardhan, and M. Brown, 2007: Evaluation of the QUIC Fast Response Dispersion Modeling System with the New York City Madison Square Garden (MSG05) Field Study: IOP 1, Release 2, draft, 47 pp.

Summary: An early version of the QUIC modeling systems was evaluated against five different types of perfluorocarbon tracers (PFTs) that were released over a 60-min period as a point-source at five different locations in the vicinity of Madison Square Garden. A scatter plot showing all gas sampler measurements for all five releases is also shown. In this study, QUIC was driven with a single non-time-varying wind which likely decreased performance. In addition, the high-rise parameterization scheme was not yet developed.

Example results:



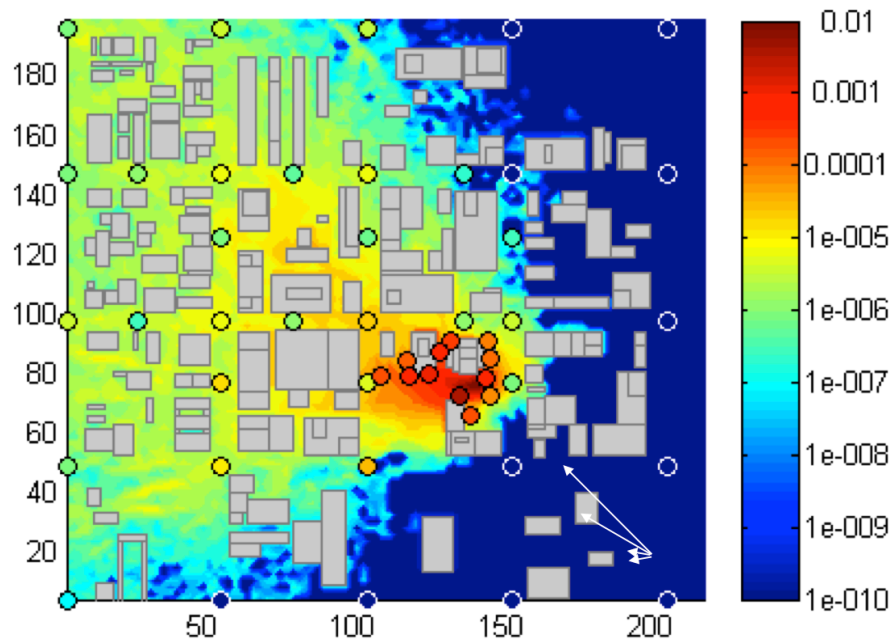
Scatter plot of computed and observed concentrations from all the release locations for the time period from 11:30am to 12:30pm. Wind direction 300° is used in QUIC simulations. Grey markers indicate measurements below the BATS sampler's LOQ specification.

5.2.4 Salt Lake City Urban 2000

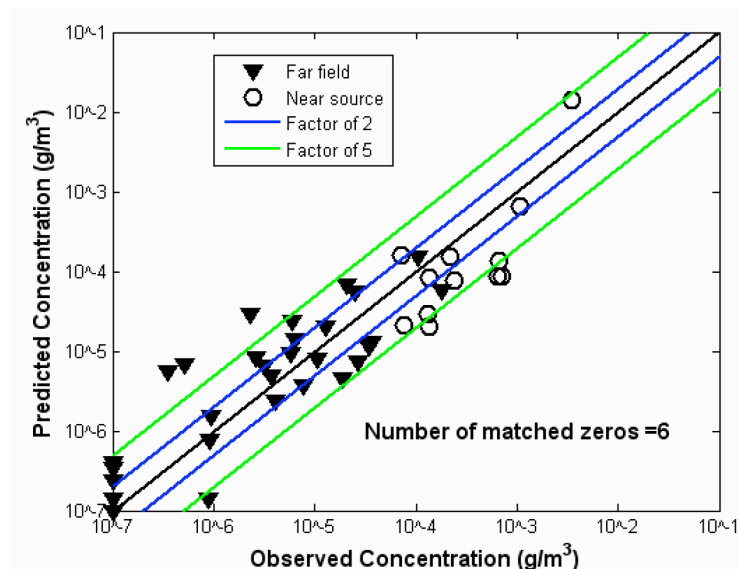
Gowardhan, A., M. Brown, M. Williams, E. Pardyjak, 2006: Evaluation of the QUIC Urban Dispersion Model using the Salt Lake City URBAN 2000 Tracer Experiment Data- IOP 10. 6th AMS Symp. Urban Env., Atlanta, GA, LA-UR-05-9017, 13 pp.

Summary: An early version of the QUIC modeling system was evaluated against SF₆ tracer measurements obtained from street-level point-source releases during the Urban 2000 field experiment in downtown Salt Lake City. Three trials during IOP 10 were evaluated and overall fairly good performance was obtained in predicting the horizontal extent of the plume. QUIC model-computed concentrations (paired both in space and in time) were within a factor of two of the measurements 42%, 52%, and 52% of the time for trials 1, 2, and 3 respectively and within a factor of five 82%, 85%, and 77% of the time.

Example results:



Comparison of one-hour-avg. SF6 bag sampler measurements (filled circles) and the QUIC-computed concentration field for IOP-10, Trial 1 (Heber-Wells release location). The wind vectors (white) depict the 15-minute averaged winds used to drive the simulation. Note the relatively good agreement in the spatial extent of the model-computed plume and the point measurements.



Scatterplot of QUIC-predicted concentrations and one-hour-avg. observed concentrations for IOP-10, Trial 1 (Heber-Wells release location).

Other sources:

Gowardhan, A., M. Brown, D. DeCroix, E. Pardyjak, 2005: Model evaluation of a fast response urban dispersion model with tracer data from the Salt Lake City Urban 2000 field experiment, *Phys. Mod. Workshop*, Ontario, Canada, 2 pp.

5.2.5 Other References

Favaloro, T., E.R. Pardyjak, M. Brown, 2007: Toward understanding the sensitivity of the QUIC dispersion modeling system to real input data, AMS 7th Symp. Urban Env., San Diego, CA, paper 10.3, 10 pp.

Gowardhan, A. and M. Brown, 2012: A study of the effects of different urban wind models on dispersion patterns using Joint Urban 2003 data, AMS 17th Conf. Appl. Air Poll. Met., New Orleans, LA.

Kastner-Klein, P. and J.V. Clark, 2004: Modeling of flow and dispersion characteristics in typical building configurations with the fast-response model QUIC, 5th AMS Urban Env. Conf., Vancouver, B.C.

Pardyjak, E.R., B. Singh, A. Norgren, and P. Willemsen, 2007: Using video gaming technology to achieve low-cost speed up of emergency response urban dispersion simulations, AMS 7th Symp. Urban Env., San Diego, CA, paper 14.2, 7 pp.

Singh, B., Pardyjak, E. R., Norgren, A., & Willemsen, P., 2011: Accelerating urban fast response Lagrangian dispersion simulations using inexpensive graphics processor parallelism. *Environmental Modelling & Software*, 26(6), 739-750.

Williams, M., M. Brown, D. Boswell, B. Singh, and E. Pardyjak, 2004: Testing of the QUIC-PLUME model with wind-tunnel measurements for a high-rise building, 5th AMS Urban Env. Conf., Vancouver, B.C., 10 pp.

Williams, M. D., M. J. Brown, and E. R. Pardyjak, 2002: Development of a dispersion model for flow around buildings, 4th AMS Symp. Urban Env., Norfolk, VA, May 20-24 2002, LA-UR-02-0839.

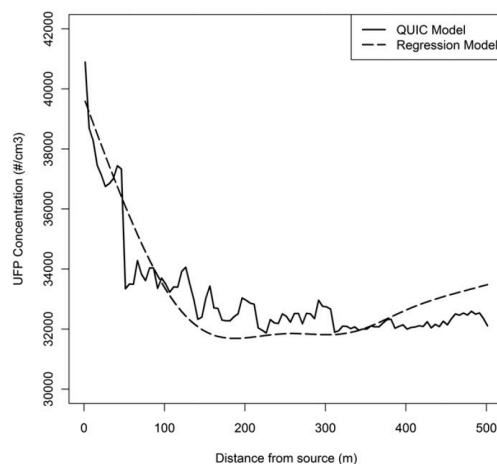
5.3 Vehicle Emissions in Cities

5.3.1 NYMETS Brooklyn Traffic Emissions Study

Zwack, L.M., S.R. Hanna, J.D. Spengler, J.I. Levy, 2011. Using advanced dispersion models and mobile monitoring to characterize spatial patterns of ultrafine particles in an urban area, *Atmospheric Environment*, 45(28), 4822-4829.

Summary: Zwack et al. (2011) independently evaluated QUIC against measurements of vehicle-emitted ultrafine particles in the Williamsburg neighborhood of Brooklyn, NY as part of NYMETS traffic study. Mobile back-pack particle monitoring devices were deployed over a three-week period including 3 hour periods during the morning and afternoon. Regressions were fit to all the measurements by the authors and used to compare how the normalized concentrations varied with distance from the primary vehicle emissions source (the Williamsburg Bridge was the only source of emissions in the QUIC modeling). The variation of the normalized concentration was fairly similar as shown in the plot below. The authors indicate that the emissions from the Williamsburg Bridge are the dominant source out to about 150 m.

Example results:



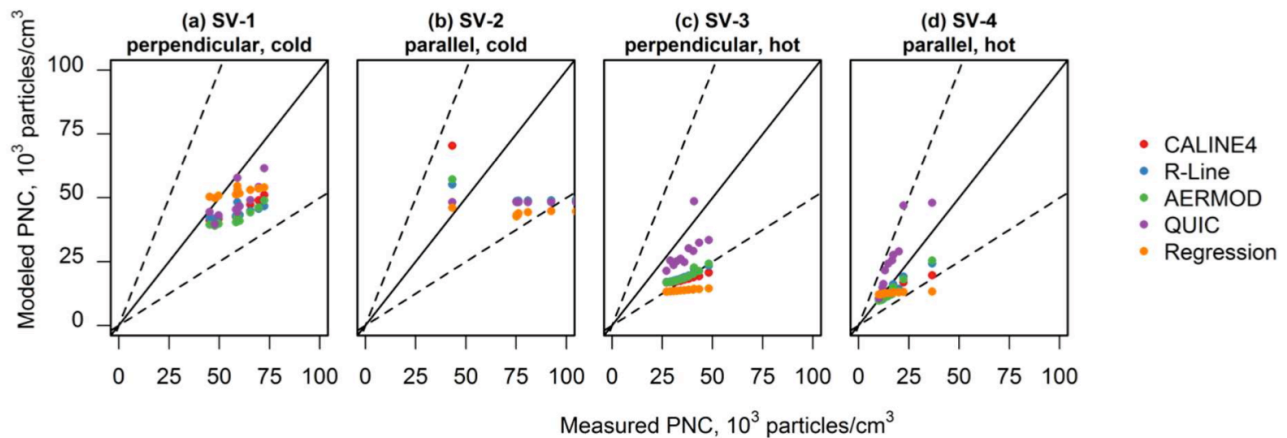
Variation of ultra-fine particle number concentration versus distance from the Williamsburg Bridge source as computed by QUIC and by regression model fit to all measurements.

5.3.2 Boston Traffic Emissions Study

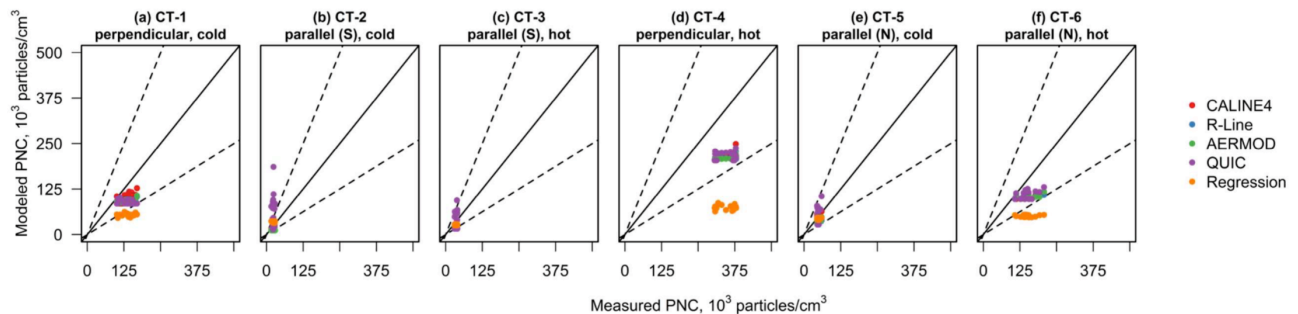
Patton, A.P., Milando, C., Durant, J.L. and Kumar, P., 2016. Assessing the Suitability of Multiple Dispersion and Land Use Regression Models for Urban Traffic-Related Ultrafine Particles. *Environmental Science & Technology*, 51(1), 384-392.

Summary: QUIC was evaluated against measurements of vehicle-emitted ultrafine particles within 200 m of highways in Sommerville, MA and in Boston's Chinatown along with three roadway plume models and a regression model. Cases were broken up into cold and hot days (resulting in different vehicle emissions and presumably different atmospheric stability, though the latter was not emphasized in the paper) and different wind directions (parallel to highway and perpendicular to the highway). Patton et al. (2016) showed that QUIC performed fairly well for most cases in Sommerville, doing best for perpendicular winds and more poorly for parallel winds. FAC2 for the four cases (see plot below) were 100, 64, 100, and 91% respectively. Results for all models were worse for Chinatown, but after modifying the background, results improved with FAC2's of 85, 40, 45, 100, 79, and 71% (see plot below). It should be noted that vehicle emissions were not measured directly, but rather estimated from assumed vehicle mix and driving characteristics and correlated to tunnel studies. In addition, only emissions from the highway were considered, but not from other nearby roadways. Authors indicate potential factors of ten uncertainty in vehicle emissions.

Example results:



Scatter plot of computed and observed particle number concentrations for Sommerville.



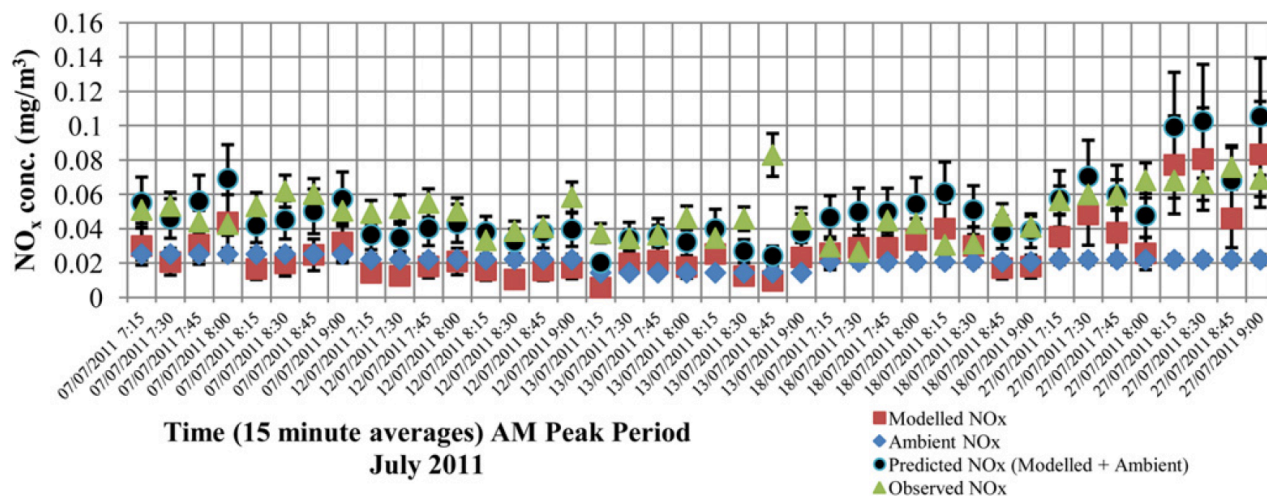
Scatter plot of computed and observed particle number concentrations for Chinatown for case of modified background.

5.3.3 Toronto Traffic Emissions Study

Misra, A., Roorda, M.J. and MacLean, H.L., 2013. An integrated modelling approach to estimate urban traffic emissions. *Atmospheric Environment*, 73, 81-91.

Summary: In an independent assessment, QUIC was evaluated against measurements of vehicle-emitted CO and NO_x in downtown Toronto during peak morning traffic (7 to 9 am) during summer months. Concentrations were obtained at one location only along a four-lane street with buildings on each side. Misra et al. (2016) showed that QUIC overpredicted CO concentration by a factor of 2 to 4, but 97.5% of QUIC-computed NO_x concentrations were within a FAC2 of the measurements. No satisfactory explanation was given by the authors for how one contaminant was apparently properly mixed and dispersed, but the other wasn't. It should be noted that a) vehicle emissions were not measured directly, but rather estimated from a microscopic emissions model; b) line source emissions in QUIC were only specified within 2 to 3 blocks of the gas sensor location (not at locations further), and c) background concentrations were obtained by using 5 am measurements.

Example results:



Comparison of computed + background concentrations (black circles) and observed concentrations (green triangles) of total nitrogen oxides for a street-level sensor in downtown Toronto.

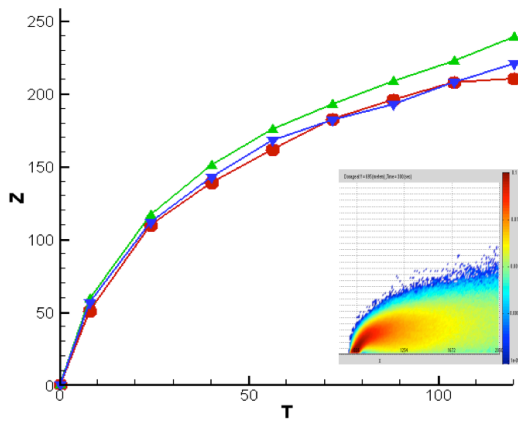
5.4 Buoyant Rise Algorithms

5.4.1 Doubletracks and Rollercoaster Explosive Rise Experiments

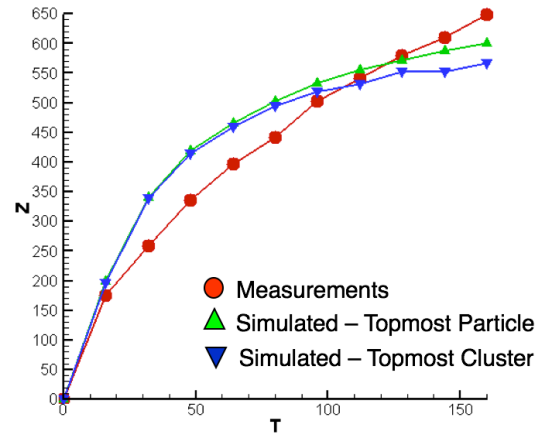
Becker, N. M., Elson, J. S., Brown, M. J., Williams, M. D., Mitchell, J. R. 2007. Radioactive Dispersive Device (RDD) Bomb Modeling in Cities for Emergency Response Using the QUIC Model. In AGU Fall Meeting Abstracts, San Francisco, CA.

Summary: The QUIC-PLUME explosive buoyant rise scheme was evaluated by comparing QUIC model output buoyant cloud top to measurements from two explosive rise experiments conducted at the Nevada Test Site. Radiosonde measurements were used to prescribe the vertical profiles of wind speed, wind direction, and temperature. Comparisons of the cloud top versus time showed very good agreement.

Example results:



Doubletracks 48 kg HE Outdoor Expt



Clean Slate 428 kg HE Outdoor Expt

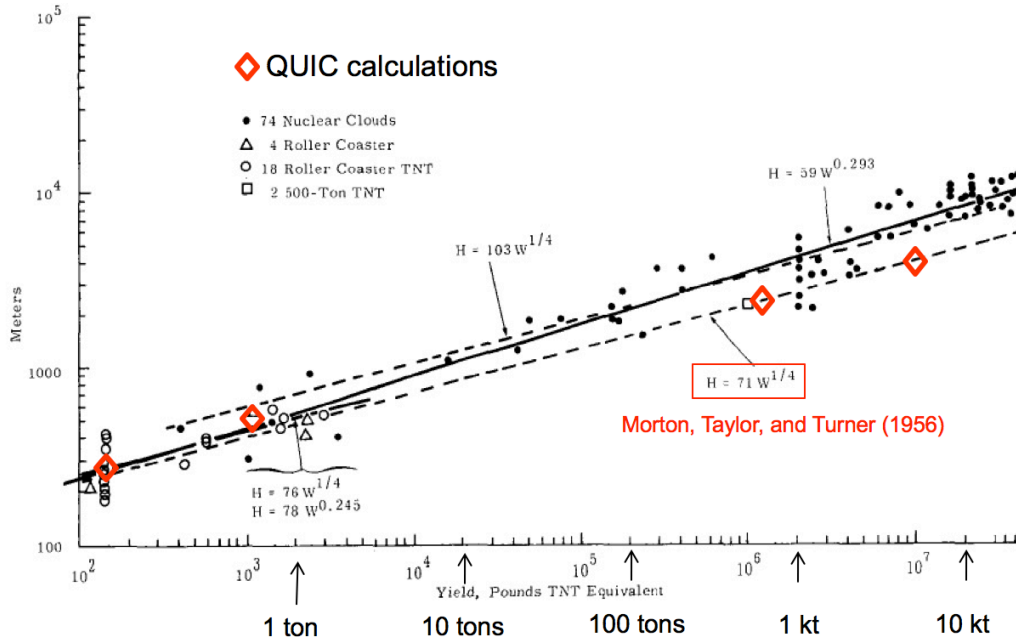
Comparison of QUIC-computed cloud top (m) versus time (s) compared to (left) the 48 kg HE Doubletracks Experiment and (right) the 428 K HE Clean Slate Experiment.

5.4.2 Church (1969) Two-Minute Cloud Top Heights

Brown, M. J., M. Williams, M. Nelson, A. Gowardhan, S. Brambilla, E. Pardyjak, 2011. *The QUIC Dispersion Modeling System: Cloud Rise, Fallout, and Modeling Issues*. JOWOG-43 Presentation, 72 pp, LA-UR-12-24176.

Summary: The QUIC-PLUME explosive buoyant rise scheme was compared to Church's (1969) summary of two-minute cloud top heights as a function of yield (expressed as TNT equivalent) and showed similar behavior, but underestimating the cloud top height for larger yields.

Example results:



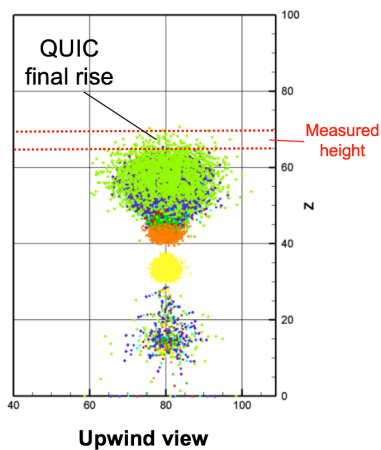
Comparison of two-minute cloud-top height measurements compiled by Church (1969) for buoyant explosive releases and QUIC-computed two-minute cloud tops (red diamonds) versus yield.

5.4.3 Morton et al. (1956) Saltwater Bubble Experiments

Brown, M. J., M. Williams, M. Nelson, A. Gowardhan, S. Brambilla, E. Pardyjak, 2011. *The QUIC Dispersion Modeling System: Cloud Rise, Fallout, and Modeling Issues*. JOWOG-43 Presentation, 72 pp, LA-UR-12-24176.

Summary: The QUIC-PLUME puff buoyant rise scheme with the entrainment algorithm turned off was compared to the Morton et al. (1956) saltwater bubble experiments. The final rise of the QUIC buoyant cloud reached a similar height as the full-scale value reported by Morton et al.

Example results:



A buoyant bubble corresponding to a 1 pound explosion of high explosive in a standard atmosphere lapse rate: the measured height is 65 to 70 meters and the QUIC final rise is similar (green particles).

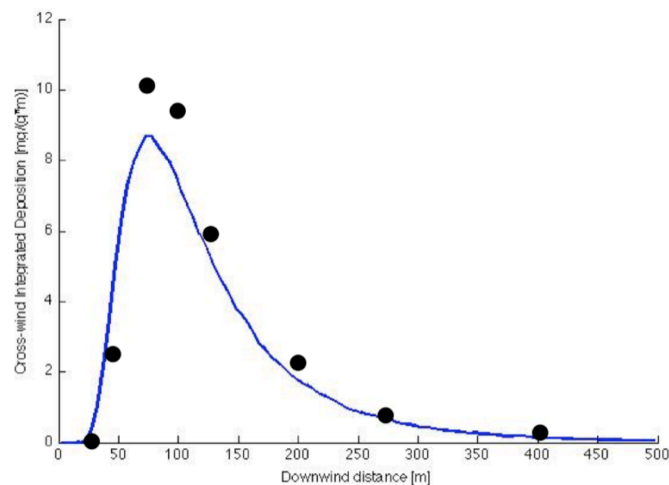
5.5 Particle Deposition

5.5.1 Walker Outdoor Glass Sphere Deposition Experiments

Zajic, D., M. Brown, M. Nelson, and M. Williams, 2011: *Description and evaluation of the QUIC wet slurry scheme: gravitational settling, droplet evaporation and surface deposition*, draft, LA-UR-10-00204, 37 pp.

Summary: Zajic et al (2011) found good agreement between QUIC-computed particle deposition and measurements taken by Walker (1965) for an elevated point-source particle release.

Example results:



A comparison of the crosswind-integrated deposition versus downwind distance measured by Walker (1965) and computed by QUIC for an elevated release of glass spheres of 56-micron mass median diameter during Trial I.

Other sources:

Zajic, D., M. Brown, M. Nelson, and M. Williams, 2010: Description and evaluation of the QUIC droplet spray scheme: droplet evaporation and surface deposition, 16th AMS Conf. Appl. Air Poll. Met., Atlanta, GA, 14 pp.

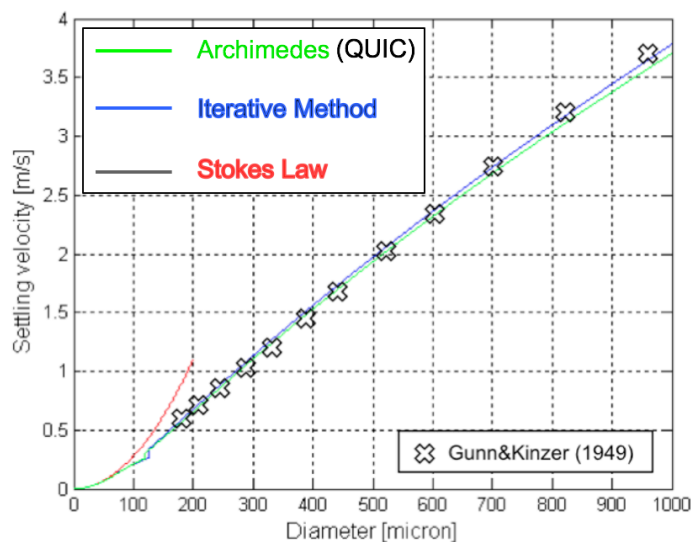
5.6 Particle Settling and Fallout

5.6.1 Gunn and Kinzer Droplet Terminal Fall Velocity Laboratory Experiments

Zajic, D., M. Brown, M. Nelson, and M. Williams, 2011: Description and evaluation of the QUIC wet slurry scheme: gravitational settling, droplet evaporation and surface deposition, draft, LA-UR-10-00204, 37 pp.

Summary: Zajic et al (2011) found good agreement between the QUIC-computed terminal fall velocity in as a function of droplet and the experimental measurements conducted by Gunn and Kinzer (1949) in stagnant air.

Example results:



Gunn and Kinzer (1949) measurements of terminal fall velocity in stagnant air as a function of droplet diameter compared to the output from the QUIC-PLUME Archimedes gravitational settling scheme, a slower iterative method, and the classic Stokes Law.

Other sources:

Zajic, D., M. Brown, M. Nelson, and M. Williams, 2010: Description and evaluation of the QUIC droplet spray scheme: droplet evaporation and surface deposition, 16th AMS Conf. Appl. Air Poll. Met., Atlanta, GA, 14 pp.

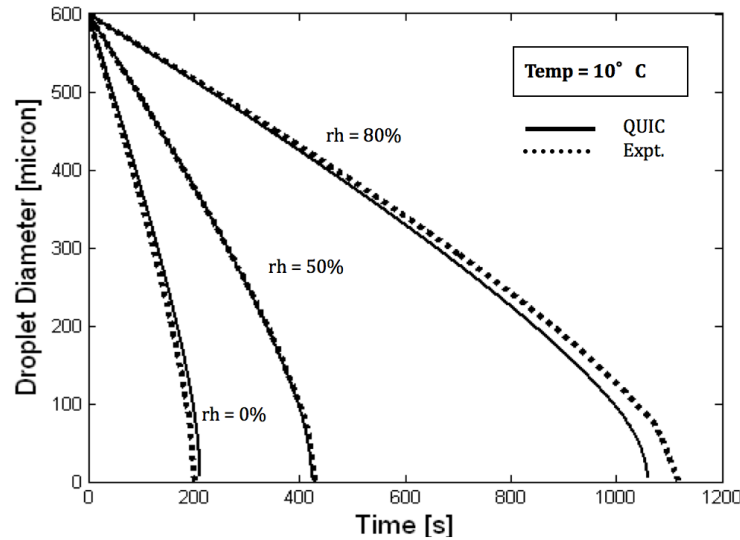
5.7 Droplet Evaporation

5.7.1 Beard and Pruppacher Droplet Evaporation Laboratory Experiments

Zajic, D., M. Brown, M. Nelson, and M. Williams, 2011: Description and evaluation of the QUIC wet slurry scheme: gravitational settling, droplet evaporation and surface deposition, draft, LA-UR-10-00204, 37 pp.

Summary: Zajic et al (2011) found good agreement between the QUIC-computed droplet evaporation as a function of time and the falling droplet laboratory measurements of Beard and Pruppacher (1971) for three different relative humidities.

Example results:



Beard and Pruppacher (1971) measurements of falling droplet evaporation as a function of time for 0, 50, and 80% relative humidity compared to the output from the QUIC-PLUME droplet evaporation scheme.

Other sources:

Zajic, D., M. Brown, M. Nelson, and M. Williams, 2010: Description and evaluation of the QUIC droplet spray scheme: droplet evaporation and surface deposition, 16th AMS Conf. Appl. Air Poll. Met., Atlanta, GA, 14 pp.

5.8 Dense Gas Transport and Dispersion

5.8.1 Thorney Island Phase 1 Trials – Flat Terrain

Brambilla, S., D. Manca, & M. Brown, 2008. Comparison of the QUIC Dispersion Model with the Thorney Island Dense Gas Trials, LANL Report, 18 pp.

Summary: Brambilla et al. (2008) ran the QUIC-PLUME dense gas modeling routines for all of the Thorney Island Phase 1 dense gas trials and found reasonable agreement between the measured and model-computed peak concentrations, although the highest peak values were typically overestimated. Using all of the samplers, roughly 74% of the model predictions were found to be within a factor of two of the measurements.

Example results:

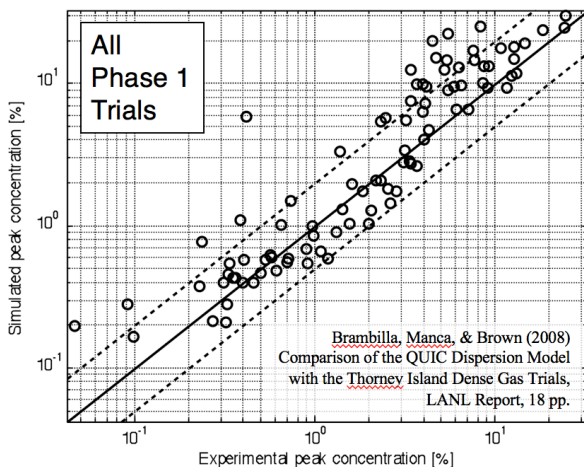


Table 6: Statistics indicators for the concentration vs. distance comparison for Phase 1

Statistics index	Literature stability classes	Best stability classes
MG	0.82	0.75
VG	1.53	1.51
FAC2 [%]	73.6	74.7

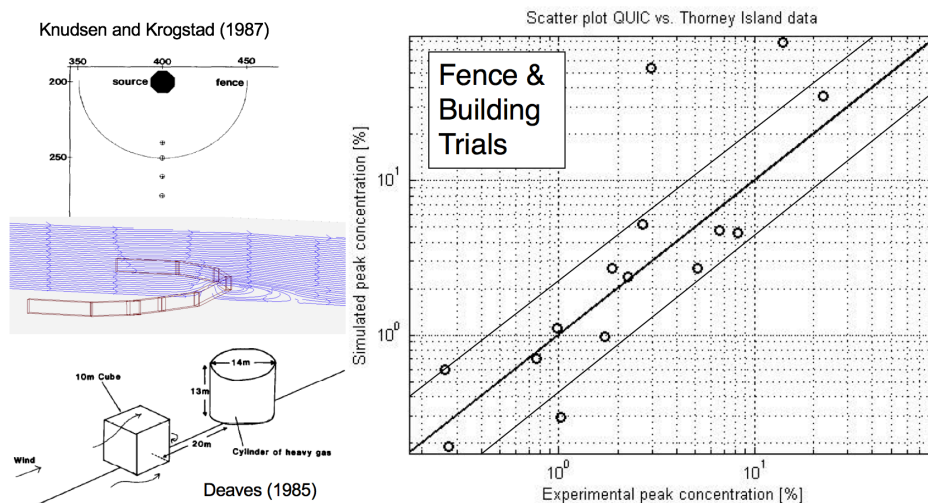
(Left) Scatterplot of the QUIC-computed and measured peak concentration for the Thorney Island dense gas instantaneous releases over flat terrain (Phase 1 Trials) and (Above) geometric mean, geometric variance, and factor of two statistics.

5.8.2 Thorney Island Phase 2 Trials – Obstacles

Brambilla, S., D. Manca, & M. Brown, 2008. *Comparison of the QUIC Dispersion Model with the Thorney Island Dense Gas Trials*, LANL Report, 18 pp.

Summary: The Thorney Island Phase 2 dense gas trials included some measurements with dense gas releases upwind of a solid fence and another a cubical building upwind of the release location. For these cases, Brambilla et al. (2008) found reasonable agreement between the measured and model-computed peak concentrations, although there were a few outlier over-predictions. Using all of the samplers, 80% of the model computed peak concentrations were found to be within a factor of two of the measurements.

Example results:



(L) Set-up of the Thorney Island solid fence and cubical building Phase 2 Trial and (R) scatterplot of simulated vs. measured peak concentrations.

Other sources:

Brambilla, S., M. D. Williams, A. Gowardhan, D. Manca, and M. J. Brown, 2009: *A shallow water model for dense gas simulation in urban areas*, AMS 8th Symp. Urban Env., Phoenix AZ, LA-UR-09-00601, 5 pp.

Williams, M., M. Brown, and A. Gowardhan, 2005: *Adaptation of the QUIC-PLUME model for heavy gas dispersion around buildings*, AMS ASAAQ San Francisco, LA-UR-05-2255, 9 pp.

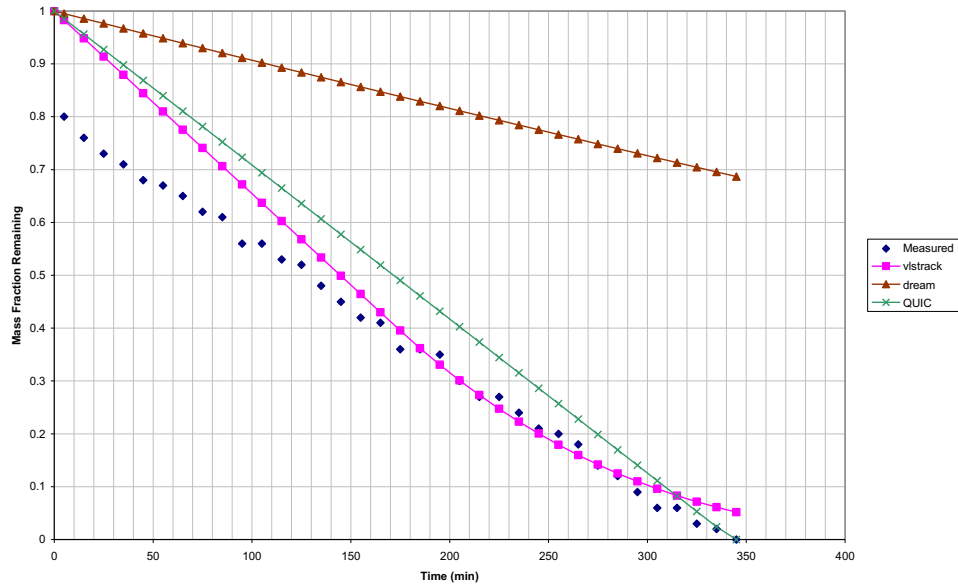
5.9 Secondary Evaporation

5.9.1 CWA Evaporation from Non-Porous Coupons

Nelson, M., M. Wolski, S. Brambilla, D. Judi, M. Brown, T. Bauer, J. Thomas, G. Dave, 2012. *Validation of Chemical Source Term Models in QUIC*, NGIC Conference, Charlottesville, VA.

Summary: Using the QUIC secondary evaporation scheme, Nelson et al. (2012) compared the model-predicted mass fraction remaining as a function of time for a GA droplet on a non-porous coupon from the experiments Agent Fate Program. The QUIC model underestimated evaporation in the first ten seconds, but the droplet lifetime was well represented.

Example results:



GA droplet mass fraction remaining versus on non-porous coupon compared to three different models. Initial rapid drop not captured, but droplet lifetime adequately predicted by VLSTRACK and QUIC.

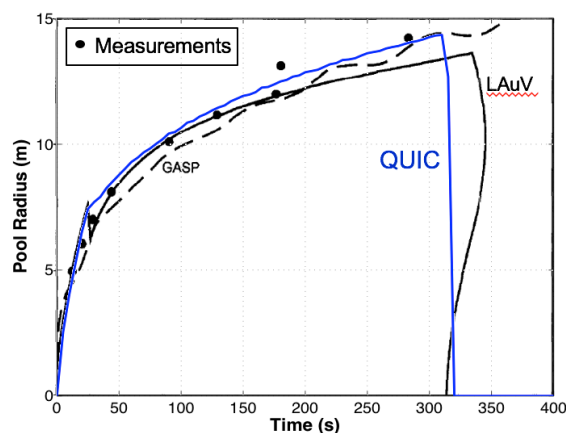
5.10 Liquid Pool Growth & Evaporation Flux

5.10.1 Liquid Natural Gas (LNG) Pool Experiment

Nelson, M., M. Wolski, S. Brambilla, D. Judi, M. Brown, T. Bauer, J. Thomas, G. Dave, 2012. Validation of Chemical Source Term Models in QUIC, NGIC Conference, Charlottesville, VA.

Summary: Using the QUIC liquid pool shallow water model with pool evaporation, Nelson et al. (2012) compared the model-predicted pool spread (radius) as a function of time to that experimentally measured in the Verfondern and Dienhart (1997) experiments. The QUIC model results lined up nicely with the measurements from the 12.5 m³ liquid natural gas release over a concrete surface.

Example results:

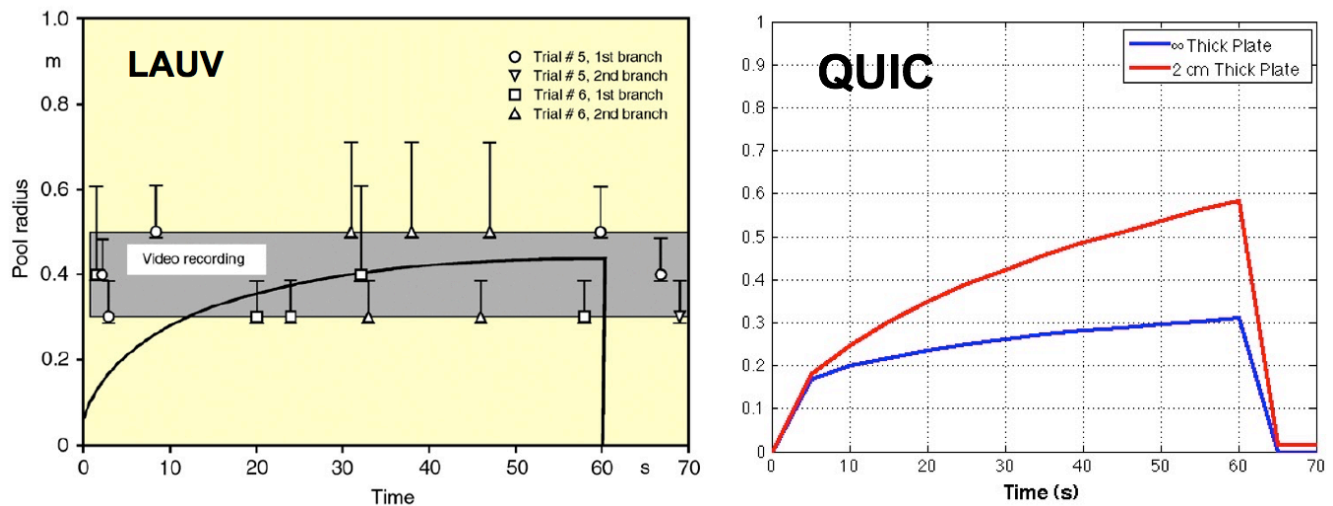


Verfondern and Dienhart (1997) measurements of pool radius as a function of time for a 12.5 m³ LNG release over a concrete surface compared to QUIC shallow water model output (blue line), as well as two other models.

5.10.2 Liquid Hydrogen Pool Experiment

Summary: Using the QUIC liquid pool shallow water model with secondary evaporation and ground cooling, Nelson et al. (2012) compared the model-predicted pool spread (radius) as a function of time to that measured in the Verfondern and Dienhart (1997) liquid hydrogen experiments on an aluminum plate. The QUIC model results for an infinitely thick aluminum plate and a 2-cm plate bounded the LAUV model result. The measurements appear to show a faster growth at the beginning as compared to both QUIC and LAUV. Both models show the cloud as completely evaporated by sixty seconds, but the measurements still show a cloud at 70s. The default infinitely thick plate assumption in QUIC matches some of the measurements on the lower end, but in general underestimates final pool growth by 25%. When QUIC is modified to account for a 2 cm plate, the model output matches some of the data on the higher end. Note: QUIC also neglects any lateral conduction within the surface.

Example results:



Verfondern and Dienhart (1997) measurements of pool radius as a function of time for a liquid hydrogen release over a 2-cm aluminum plate compared to (left) the LAUV pool spread model and (right) the QUIC shallow water liquid pool model output with the default infinitely thick plate and a specially-adapted 2-cm thick plate.

Verfondern & Dienhart 2007: Pool spreading and vaporization of liquid hydrogen. Int. J. of Hydrogen Energ., 32, 256-267.